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NON-ITERATIVE GEOMETRIC APPROACH TO NONLINEAR PARAMETRIC
LEAST-SQUARES ADJUSTMENT WITH OR WITHOUT CONSTRAINTS

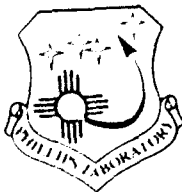
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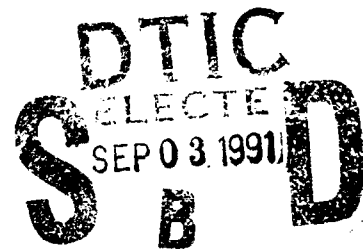
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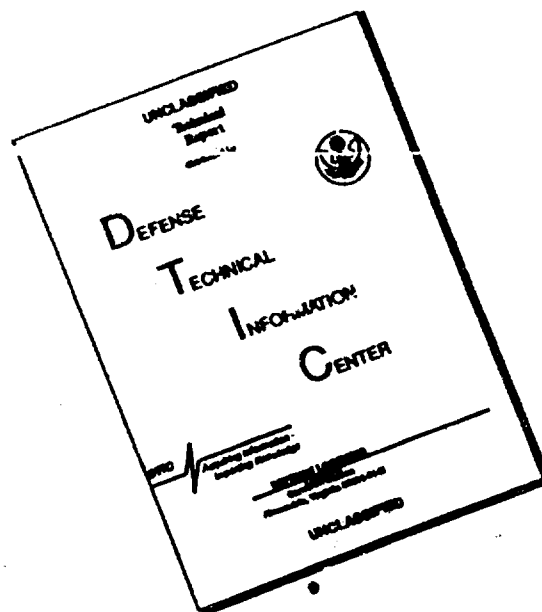


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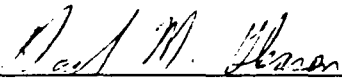


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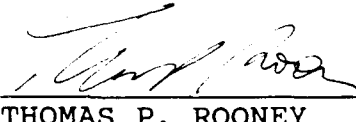


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| <p>A nonlinear parametric adjustment model with n observations and u parameters can be interpreted geometrically as the description of a u-dimensional "model surface" embedded in an n-dimensional flat "observational space". Two geometric concepts have been identified for the least-squares resolution of this model. The first concept is linked to the Gauss form of the surface, which is the most direct representation of the parametric model; however, the solution is iterative in nature. The second concept is linked to the functional form of the surface, and it leads to a non iterative solution.</p> | | |

The Gauss form of the surface is presented as

$$x^r = x^r(u^\alpha), \quad r = 1, 2, \dots, n, \quad \alpha = 1, 2, \dots, u,$$

where x^r are the space coordinates and u^α are the surface coordinates of points lying in the surface. Upon identifying the observations with the observational-space coordinates of the point Q, the least-squares solution is seen to correspond to the point P in the model surface such that the distance QP is a minimum. Accordingly, the vector PQ is orthogonal to the model surface.

The Gauss form can be transformed into the functional form of the surface:

$$F^L(x^r) = 0, \quad r = 1, 2, \dots, n, \quad L = 1, 2, \dots, n-u,$$

where the superscript L distinguishes $n-u$ functions "F" one from another. This formulation, where $n-u$ represents the number of degrees of freedom, can be linked to the condition method of adjustment with a very special set of functions "F". A readily perceived advantage of the functional form is that the $n-u$ gradients of these "F" are vectors orthogonal to the model surface, which is instrumental in expressing the final vector PQ.

Both concepts make use of the Taylor-series expansion containing the first- and higher-order partial derivatives of the observables with respect to the parameters. In the Gauss-form approach, the derivatives can be used at most up to the third order. In principle, such a truncation of the Taylor series results in the necessity to iterate the solution. In the functional-form approach, the number of useful terms in the Taylor series has no limitation, and can be chosen such that the final outcome is determined with sufficient accuracy in a single step. This approach is the subject of a detailed study.

The role of eventual nonlinear constraints in both geometrical approaches is to restrict the model surface to a "model subsurface", but otherwise no conceptual modification takes place. Accordingly, the resulting nonlinear adjustment model contains a reduced number of parameters. From this point on, the treatment of the new model is indistinguishable from the treatment of the original model without constraints.

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TABLE OF CONTENTS

| | Page |
|---|------|
| 1. INTRODUCTION | 1 |
| 2. ELEMENTS OF THE MATHEMATICAL BACKGROUND | 3 |
| 3. FUNCTIONAL-FORM APPROACH TO NONLINEAR PARAMETRIC LEAST-SQUARES ADJUSTMENT | 8 |
| 3.1 Two Geometrical Concepts Reflecting the Least-Squares Methodology | 8 |
| 3.2 Overview of the Functional-Form Concept | 11 |
| 4. DEVELOPMENT OF THE FUNCTIONAL-FORM APPROACH IN FOUR STEPS | 17 |
| 4.1 First-Step Derivation | 17 |
| 4.2 Q-Surface Determination | 20 |
| 4.3 Third and Fourth Steps | 23 |
| 5. VARIANCE-COVARIANCES AND OTHER ADJUSTMENT QUANTITIES | 33 |
| 6. DISCUSSION | 39 |
| 6.1 Relation to the Condition Method | 39 |
| 6.2 Solution for a Linear Model | 40 |
| 7. CONCLUSION | 42 |
| APPENDIX A: NUMERICAL EXAMPLE | 45 |
| APPENDIX B: PARAMETRIC ELIMINATION DUE TO NONLINEAR CONSTRAINTS | 52 |
| B.1 Initial Parametric Values | 52 |
| B.2 Model Subsurface | 54 |
| B.3 Modified Nonlinear Model with a Reduced Number of Parameters | 57 |
| REFERENCES | 60 |

LIST OF FIGURES

| | Page |
|--|------|
| 1. THREE DIMENSIONAL REPRESENTATION OF ISOMORPHIC LEAST-SQUARES SOLUTION | 10 |
| 2. GENERATION OF A TWO-DIMENSIONAL Q-SURFACE FROM A TWO-DIMENSIONAL MODEL SURFACE | 15 |
| 3. GENERATION OF A ONE-DIMENSIONAL Q-SURFACE FROM A ONE-DIMENSIONAL MODEL SURFACE | 16 |

1. INTRODUCTION

A series of studies linking an adjustment model to a geometrical setup with tensor structure and notation began with [Blaha, 1984]. However, that report treated a linear or linearized adjustment model; a nonlinear model would in general entail an iterative process. A more recent study, [Blaha, 1989a], contained a geometrical development of an accelerated iterative process taking advantage of the second- and third-order partial derivatives (at the most) of the observables with respect to the parameters, in addition to the usual first-order partial derivatives featured by the linearized model. The present study, by contrast, describes a non-iterative approach, where advantage can further be taken of the fourth- and possibly higher-order partial derivatives. In addition to its theoretical interest, this approach enables one to resolve problems where fourth-order partial derivatives are significant and cause difficulties in alternate adjustment schemes.

The approach is based on the Taylor-series expansion of the observables in terms of the parameters, and on the geometrical concept, generalized to higher dimensions, that the gradient of the potential at a given point is orthogonal to an equipotential surface at that point. We emphasize that whenever an adjustment is mentioned, it is the least-squares adjustment that we have in mind. In geometrical terms, this implies the generalized notion of the shortest distance from a surface, and of the associated orthogonality. Indeed, the least-squares principle has provided the motivation for interpreting adjustment models, linear or nonlinear, with or without constraints, in a generalized context.

The mathematical background needed in relating nonlinear parametric adjustment to geometry is presented in Chapter 2. Parts of this material are common to some of the previous reports, and have appeared in Chapters 1 and 2 of [Blaha, 1989a], and in Chapter 2 of [Blaha, 1989b]. However, their recapitulation is useful for the development of a new approach, referred to as the functional-form approach, in the body of the present study. The "functional form" derives its name from the manner in which we express the "model surface"; the latter is in general a hypersurface representing the adjustment model in its geometric analogy. The resulting algorithm has been implemented on a personal computer, and verified using the adjustment problem of Appendix A in [Blaha,

1989a], formulated in terms of a third-degree polynomial in four variables. The outcome of this verification is presented in Appendix A herein.

The method developed for non-iterative adjustment of a nonlinear parametric model can be used whether or not there exist constraints among the parameters. In the adjustment context, the presence of s constraints can be used to eliminate s parameters. In the geometrical context, the s constraints restrict the u -dimensional model surface to an embedded $u-s$ dimensional "model subsurface". With the exception of the model subsurface taking place of the original surface, the geometrical concept remains unaltered. Indeed, from this point on, the treatment of the new model is indistinguishable from the treatment of the original model, whether by the method developed herein or by the methods of [Blaha, 1989a]. The restriction of the model surface to the model subsurface, and its algorithmic realization, are the subject of Appendix B, which represents an expanded version of Sections 3.1 and 3.2 in [Blaha, 1989b].

2. ELEMENTS OF THE MATHEMATICAL BACKGROUND

The parametric adjustment model expresses each of the observables in terms of parameters, where the structure linking the two groups of variables is, in general, nonlinear. The number of observables is denoted by n and the number of parameters by u , where n must be greater than u for an adjustment to take place. In matrix notation, the adjustment model is written as

$$L^a = F(X^a) ,$$

where L^a and X^a are the sets (column-vectors) of adjusted observations and adjusted parameters, respectively. Such estimates are always considered to be consistent with the least-squares principle.

In a standard adjustment approach, a nonlinear adjustment model is subject to the Taylor-series expansion based on an initial set of parametric values, X^0 . The terms in the second and higher powers of the parametric corrections are neglected, resulting in the well-known (linearized) observation equations. In matrix notation, the latter are expressed by

$$V = A X + L ,$$

where A is the design matrix, $X = X^a - X^0$ is the column-vector of parametric corrections, $V = L^a - L^b$ is the column-vector of residuals, and $L = L^0 - L^b$ is the column-vector of constant terms, with $L^0 = F(X^0)$ representing observables consistent with the initial set of parameters, and L^b containing the actual observations. The linearized model is subjected to the least-squares criterion

$$V^T P V = \text{minimum} ,$$

where P is the weight matrix of observations. This criterion leads to the formation of the familiar normal equations.

If the original adjustment model is nonlinear, the resolution of the linearized model does not yield the final answers. The process is usually repeated with new, updated parameters and the corresponding changes in A and L . However, the variance covariance matrix of observations, Σ , as well as the weight matrix P , adopted as $P = \Sigma^{-1}$, are constant. Thus, the matrix of normal equations, $N = A^T P A$, changes only due to A , and the column vector representing the right hand side of normal equations, $U = A^T P L$, changes only due to A and L .

The computation of the updated parametric values through a new X requires the formation and the inversion of a new N in each iteration, or a mathematically equivalent procedure. When X becomes sufficiently close to zero the iterative process is terminated. As its by-product, the latest matrix N^{-1} is adopted as the variance-covariance matrix of adjusted parameters.

The functional relationship between the observables and the parameters lends itself to a geometrical interpretation and treatment involving spaces and surfaces generalized to higher dimensions. In particular, the formulation

$$x^r = x^r(u^\alpha), \quad r = 1, 2, \dots, n, \quad \alpha = 1, 2, \dots, u,$$

representing the parametric adjustment model, can be linked to the Gauss form of a surface in relation to the surrounding space, where x^r are the space coordinates and u^α are the surface coordinates. The Gauss form of a two-dimensional surface ($u=2$) embedded in a three-dimensional flat space ($n=3$) is described, together with two other forms, in Chapter 6 of [Hotine, 1969]. In [Blaha, 1984], both the n -dimensional "observational" space and the u -dimensional "model" surface were considered flat. The latter was thus in reality a hyperplane. Although the model surface is now intrinsically a curved space, the surrounding space is again flat, and, as is shown below, its coordinate system is characterized by a constant metric tensor.

In denoting the n observables by x^r , $r=1, 2, \dots, n$, and the u unknown parameters by u^α , $\alpha=1, 2, \dots, u$, we can represent a nonlinear parametric adjustment model by

$$\begin{aligned} x^r = x^r(u^\alpha) = x_0^r + \Lambda_\alpha^r \Delta u^\alpha + (1/2) \Omega_{\alpha\beta}^r \Delta u^\alpha \Delta u^\beta \\ + (1/6) \Phi_{\alpha\beta\gamma}^r \Delta u^\alpha \Delta u^\beta \Delta u^\gamma + \dots \end{aligned} \quad (1a)$$

$$\Delta u^\alpha = u^\alpha - u_0^\alpha, \quad (1b)$$

where u_0^α represents an initial set of parameters and $x_0^r = x^r(u_0^\alpha)$ represents the observables consistent with this set. The lower-case Roman indices range from 1 to n , and the lower-case Greek indices range from 1 to u . Tensor symbolism implies the summation convention over the dummy (repeating) indices.

In the geometrical context, the first equality in (1a) represents the Gauss form of a u dimensional surface embedded in an n dimensional space. The surface is endowed with the coordinate system $\{u^\alpha\}$, $\alpha=1, 2, \dots, u$ and is referred to as

the model surface, and the space is endowed with the coordinate system $\{x^r\}$, $r=1,2,\dots,n$, and is referred to as the observational space. The second equality in (1.1) is the Taylor series expansion of x^r from the "initial" point P lying in the model surface, whose model-surface coordinates are u_0^α and whose observational-space coordinates are x_0^r . The notation identifying the partial derivatives at P , such as $\partial x^r / \partial u^\alpha \equiv A_\alpha^{r0}$, $\partial^2 x^r / \partial u^\alpha \partial u^\beta \equiv \Omega_{\alpha\beta}^r$, etc., is self-evident. The actual observations can be thought of as describing the point Q in the observational space, which, due to measuring errors, does not lie in the known model surface. The task at hand consists in determining, from the observed point Q , a model-surface point satisfying the least-squares criterion

In the adjustment context, the variance-covariance and the weight matrices of observations depend on the quality of measurements. They are independent of the adjustment model, of the initial set of parameters, of the outcome of observations, etc. Thus, for a given observational mode they are constant. In the "traditional" identification of [Biaha, 1984], variance covariance matrices correspond to associated metric tensors, and weight matrices correspond to metric tensors. Accordingly, we represent the variance-covariance matrix of observations by the observational-space associated metric tensor g^{rs} , and the weight matrix of observations by the observational-space metric tensor g_{sr} , and state that both tensors are independent of the form of the model surface, of the initial point P , of the observed point Q , etc., leading to the simplification

$$g_{sr} = \text{constant} . \quad (2)$$

One could also attribute the tensors g^{rs} and g_{sr} to the point Q and state that the geometrical setup must account for Q located anywhere in the observational space. In turn, (2) implies that the observational space must be flat.

If the set δx^r denotes the coordinate differences between the observed point Q and the desired model-surface point denoted \bar{P} , it corresponds to the negative residuals, and the least-squares criterion corresponds to

$$\delta S^2 = \delta x^s g_{sr} \delta x^r = \text{minimum} . \quad (3)$$

The quadratic form (3) represents the square of the distance between Q and \bar{P} . Therefore, the desired "least-squares" point \bar{P} must be the foot-point of the straight line dropped orthogonally from Q onto the model surface. We note that if any other adjustment condition were used in lieu of the least-squares

criterion, the minimum-distance property (3) would not exist and the geometric-tensorial treatment of the adjustment theory would probably be much more complex if not impossible.

A convenient approach for resolving nonlinear least-squares problems consists in using an isomorphic geometrical setup with tensor structure and notation. Such a link is highlighted by the consideration that the least-squares criterion gives rise to a minimum-distance property. Among the basic correspondences, the number of observations, n , and the number of parameters, u , define the dimensionality of the observational space and of the model surface, respectively. Since the constant variance-covariance matrix of observations, Σ , corresponds to the associated metric tensor g^{rs} , and the weight matrix of observations, adopted as Σ^{-1} , corresponds to the metric tensor g_{sr} , the observational space is endowed with a coordinate system $\{x^r\}$ such that

$$g_{sr} = \text{constant}, \quad g^{rs} = \text{constant}.$$

The set L^b of actual observations corresponds to the set x_Q^r of observational-space coordinates describing the point Q . All possible sets of adjusted observations (subject to no criterion) correspond to the Gauss form of the model surface endowed with a coordinate system $\{u^\alpha\}$, which has already appeared above:

$$x^r = x^r(u^\alpha), \quad r = 1, 2, \dots, n, \quad \alpha = 1, 2, \dots, u.$$

The final set of adjusted parameters, X^a , corresponds to a particular set u^α of model surface coordinates describing the least-squares point \bar{P} . The set of initial parameters, X^0 , corresponds to the set u_0^α of model-surface coordinates describing the initial point P . The final set of parametric corrections, X , then corresponds to $\Delta u^\alpha = u^\alpha - u_0^\alpha$; these quantities are assumed to be small. The final set of adjusted observations, $L^a = F(X^a)$, corresponds to a particular set $x^r = x^r(u^\alpha)$ of observational-space coordinates describing the least squares point \bar{P} . The initial point P is described by these coordinates as $x_0^r = x^r(u_0^\alpha)$, reflecting its counterpart $L^0 = F(X^0)$. The set of negative constant terms, $-L = L^b - F(X^0)$, corresponds to the contravariant vector $\delta x^r = x_Q^r - x_0^r$, while the set of negative residuals, $-V = L^b - L^a$, corresponds to the contravariant vector $\delta x^r = x_Q^r - x^r$. The initial design matrix, A , which in standard observation equations, $V = AX + L$, relates the parametric corrections to the residuals, corresponds to the design tensor $A_\alpha^r = \partial x^r / \partial u^\alpha$ evaluated at P .

On the other hand, the standard adjustment approach does not have equivalents of the above $\Omega_{\alpha\beta}^r$ and $\Phi_{\alpha\beta\gamma}^r$, which form three- and four-dimensional arrays, respectively, and contain the second- and the third-order partial derivatives of x^r with respect to u^α , evaluated at P .

We further comment that the surface associated metric tensor at \bar{P} corresponds to the variance-covariance matrix of adjusted parameters, and the "necessary" version of the space associated metric tensor at \bar{P} corresponds to the singular variance-covariance matrix of adjusted observations. Such correspondences, as well as the definition of "necessary" tensors, were presented in Sections 2.2 and 4.2 of [Blaha, 1984]. (A better term might be "restricted", in the sense of a restriction to the hyperplane tangent to the model surface at \bar{P} .) In the same vein, the surface metric tensor at \bar{P} corresponds to the weight matrix of adjusted parameters, and the "necessary" version of the space metric tensor at \bar{P} corresponds to the singular weight matrix of adjusted observations.

These notions confirm the variance-covariance propagation law and introduce a "weight propagation law", and they can be extended to functions of adjusted parameters as well as to functions of adjusted observations. In [Blaha, 1984], however, they were demonstrated only for linear models. In nonlinear models the above tensors, expressible by means of orthonormal vectors tangent to the model surface at \bar{P} , could be said to describe tangential, or first-order, properties of least-squares estimates. In the present study, the derivation of the metric tensors corresponding to the weight matrices will be by-passed, and only the derivation of the associated metric tensors corresponding to the desired variance-covariance matrices will be carried to term. This also implies that the formation of the weight matrix of observations (by inverting their variance-covariance matrix) will be by-passed.

3. FUNCTIONAL-FORM APPROACH TO NONLINEAR PARAMETRIC LEAST-SQUARES ADJUSTMENT

3.1 Two Geometrical Concepts Reflecting the Least-Squares Methodology

In the preceding chapter, we have seen that a nonlinear parametric adjustment model with n observations and u parameters can be interpreted geometrically as the description of a u -dimensional "model surface" embedded in an n -dimensional flat "observational space". The most direct interpretation is linked to the Gauss form of the surface:

$$x^r = x^r(u^\alpha) , \quad r = 1, 2, \dots, n , \quad \alpha = 1, 2, \dots, u ,$$

where x^r are the space coordinates and u^α are the surface coordinates of points lying in the surface. Upon identifying the observations with the observational space coordinates of the point Q , the least-squares solution corresponds to the point \bar{P} in the model surface such that the distance $Q\bar{P}$ is a minimum. Accordingly, the vector $\bar{P}Q$ is orthogonal to the model surface.

In a separate representation as treated in the present study, one can transform the Gauss form into the functional form:

$$F^L(x^r) = 0 , \quad r = 1, 2, \dots, n , \quad L = 1, 2, \dots, n-u ,$$

where the superscript L distinguishes $n-u$ functions "F" one from another. This formulation, where $n-u$ represents the number of degrees of freedom, can be linked to the condition method of adjustment with a very special set of functions F^L . A readily perceived advantage of the functional form is that the $n-u$ gradients of F^L are vectors orthogonal to the model surface, which is instrumental in expressing the final vector $\bar{P}Q$.

Both of the above concepts can be applied to the nonlinear parametric least-squares adjustment, where use is made of the Taylor series expansion containing the first- and higher-order partial derivatives of the observables with respect to the parameters. In the Gauss form approach developed in [Blaha, 1989a], the partial derivatives can be used at most up to the third order. In principle, such a truncation of the Taylor series results in the necessity to iterate the solution, but this process converges much faster than would be the case with the linearized model. On the other hand, in the functional-form approach developed herein, the number of useful terms in the Taylor series has

no limitation and can be chosen such that \bar{P} is determined with sufficient accuracy in a single step.

Independent of the model-surface formulation, the least-squares principle is illustrated in Fig. 1. This illustration is limited in that $n=3$ (the observational space is three dimensional), $u=2$ (the model surface is two dimensional), and $L=1$ ($L=n-u$). The unbarred quantities in the figure are associated with the known "initial point" P , while the barred quantities are associated with the desired "least-squares point" \bar{P} ; both P and \bar{P} lie in the model surface. The vector ν of the orthonormal triad ℓ, j, ν is orthogonal to this surface, with a similar construction applying for \bar{P} and other surface points.

In the absence of observational errors, the "observational point" Q would lie in the model surface. (In the algebraic formulation, the system of observation equations would be consistent and there would be no need for an adjustment.) From the geometric point of view, an optimal estimate of a hypothetical, error-free observational point is that point in the model surface which is the closest to the actual point Q . Thus, the line connecting Q with this closest point, which is \bar{P} by construction, is necessarily orthogonal to the model surface. This is illustrated in Fig. 1 by the colinearity of the vectors $\bar{P}Q$ and $\bar{\nu}$.

Since, as has been discussed in Chapter 2, the metric tensor of the observational space is constant due to the nature of the parent adjustment setup (the weight matrix of observations is independent of the mathematical model, the initial values of the parameters, the numerical outcome of the observations, etc.), we have

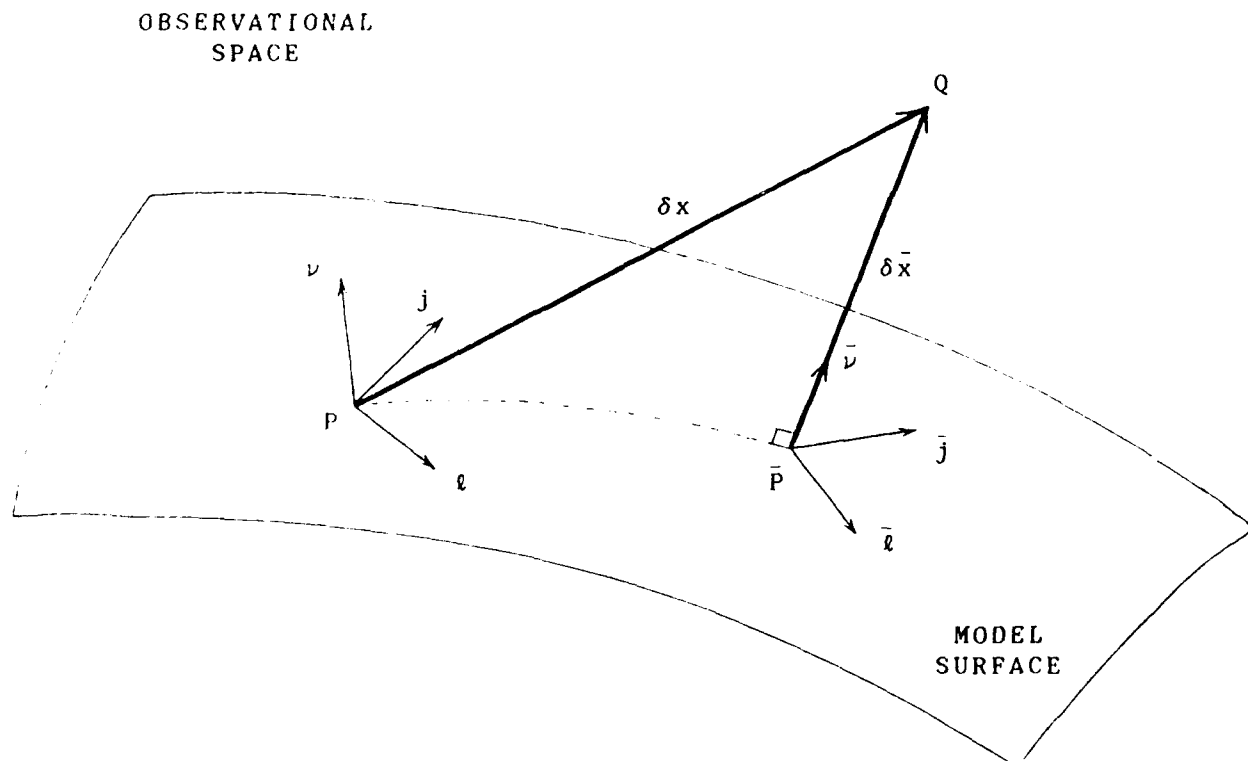
$$\bar{g}_{sr} = g_{sr} = \text{constant} .$$

Accordingly, the space Christoffel symbols are zero and the space covariant derivatives are simply the partial derivatives. The above-mentioned optimal estimate has been seen in (3) to correspond to

$$\delta \bar{x}^s g_{sr} \delta \bar{x}^r = \text{minimum} .$$

where the summation convention for the repeating (dummy) indices applies. This relation, associated with the point \bar{P} , expresses the least-squares criterion.

THREE-DIMENSIONAL REPRESENTATION
OF ISOMORPHIC LEAST-SQUARES SOLUTION



GIVEN PROPERTY: $\bar{g}_{sr} = g_{sr} = \text{constant}$

LEAST-SQUARES CRITERION IN TENSOR NOTATION:

$$\delta \bar{x}^s g_{sr} \delta \bar{x}^r = \text{minimum}$$

VECTOR $\delta \bar{x}$ IS ORTHOGONAL TO THE MODEL SURFACE AT \bar{P}

DEPICTING THE LEAST-SQUARES SOLUTION

Fig. 1

3.2 Overview of the Functional-Form Concept

In accordance with the foregoing, a least-squares problem can be viewed as the task of drawing a geodesic (a straight line in the flat observational space) through a known observational point Q orthogonally to a given model surface. The intersection of the geodesic with the model surface marks the desired least squares point P. In the functional form approach, this task is solved by designing a geodesic orthogonal to the model surface through the initial point P, by implicitly evaluating the miss of the "target" Q by this line, and by displacing the point P in the model surface in such a way that the new geodesic (again orthogonal to the model surface) passes through the target.

The functional-form approach can be described as consisting of four steps. In the first step, the equations of the model surface are transformed from the Gauss form to the functional form via the Monge form, leading to the expressions for the (space) gradient vectors associated with the model surface, and their derivatives. In this process, the familiar geometrical concepts are extended to a u-dimensional surface embedded in an n-dimensional space. The space coordinates are divided into the group encompassing the first u coordinates, identified by the lower-case Greek indices, and into the group encompassing the last n-u coordinates, identified by the upper-case Roman indices. Accordingly, the Gauss form of the model surface,

$$x^r = x^r(u^\beta) , \quad r = 1, 2, \dots, n , \quad \beta = 1, 2, \dots, u , \quad (4)$$

where u^β represents the (original) model-surface coordinates, is written as

$$x^\alpha = x^\alpha(u^\beta) , \quad (5a)$$

$$x^L = x^L(u^\beta) . \quad (5b)$$

If the set of partial derivatives $\partial x^\alpha / \partial u^\beta$ forms a regular (i.e., square and nonsingular) matrix, $\{x^\alpha\}$ will be adopted as a new set of model-surface coordinates. In addition to representing the first u space coordinates. The inverse transformation between the two model-surface coordinate systems is symbolized by

$$u^\beta = u^\beta(x^\alpha) . \quad (6a)$$

The substitution of (6a) into (5b) yields the Monge form of the model surface:

$$x^L = x^L(u^\beta(x^\alpha)) \equiv f^L(x^\alpha) , \quad (6b)$$

where the index L (or another upper-case Roman index) attributed to f distinguishes the n-u functions one from another. Finally, the functional form of the model surface follows from (6b) as

$$x^L - f^L(x^\alpha) = F^L(x^r) = 0 , \quad (7)$$

where the index L attributed to F has a role similar to that just mentioned. In a three-dimensional space containing a two-dimensional surface, (7) would correspond to one equation $F(x^r)=0$, such as $F(x,y,z)=0$ in space Cartesian coordinates, whereas in the general case being developed the number of equations is n-u.

In general, the functional form based on (7) is represented by

$$F^L(x^r) = N^L - \text{constant} , \quad (8)$$

where "constant" represents a set of n-u constants. The zero value of these constants identifies the model surface, as is apparent from (7). Here again, L (or another upper-case Roman index) distinguishes the scalar functions of position, N, one from another, so that its role is to account for all of the n-u functions N. The same logic is utilized when describing the gradients and higher-order derivatives of these functions. Thus, if N_r is the gradient of N, the notation N_r^L symbolizes the entire set of n-u gradients. The advantage of the formulation (8) is that each of the gradients N_r is orthogonal to the pertinent surface, in the sense that $N_r^L k^r = 0$, where k^r is any contravariant vector (i.e., a vector identified by its contravariant components) tangent to the surface. This orthogonality property is crucial, since, as we have seen, the known observational point Q must lie on a line drawn from the least-squares point \bar{P} orthogonally to the model surface.

In addressing this task, one might be tempted to generate a family of surfaces in space, each of which would be described by the functional form (8) with a given set of constants. (When these constants are zero, we recover the model surface.) We could stipulate that one member of the family contains the point Q, and could determine its set N^L . However, this avenue presents a major difficulty, in that the determination of intersections of straight lines, orthogonal to the model surface, with the new surface amounts to solving a nonlinear system of equations. This difficulty has been mentioned merely to

illustrate that the popular concept of a family of surfaces does not advance our task, and that we shall have to resort to an unorthodox definition of a surface as is explained below.

The second step of the new approach defines a special "Q-surface" containing the point Q. However, one can describe this surface only by construction and not by defining equations. In particular, a point of the Q-surface is generated in the observational space from a chosen model-surface point, for example from the initial point P. First, we conceive of n-u straight lines drawn from P, which are orthogonal to the model surface and form an n-u dimensional hyperplane. And second, this hyperplane is intersected by a straight line which is orthogonal to it and passes through the point Q. The intersection, denoted \tilde{P} , generates a point of the Q-surface. In considering the correspondence between a general point P in the model surface and its counterpart \tilde{P} in the Q surface, we confirm that the point Q itself is the counterpart of \tilde{P} .

The above construction can be illustrated in the familiar context of a three-dimensional space containing a two-dimensional surface, where only one straight line perpendicular to the model surface would emanate from P. This line, representing a one-dimensional "hyperplane", would be intersected by a straight line drawn perpendicularly to it from Q, which would generate a point of the Q-surface. Such a situation is depicted in Fig. 2, where the generated point is denoted \hat{P} as above, and v is a vector orthogonal to the model surface at P.

We can imagine a similar situation, illustrated in Fig. 3, in terms of a one-dimensional "surface" (i.e., a line) embedded in a three-dimensional space. There would now be two vectors emanating from P, in Fig. 3 denoted v' and v'' , which would be perpendicular to this "surface" and would generate a "hyperplane" (here a plane); such vectors are referred to as vectors v . The straight line dropped perpendicularly from Q onto this "hyperplane" would then generate a point of the Q-"surface", denoted again \tilde{P} .

The construction of \tilde{P} shows that the vector $P\tilde{P}$ is the orthogonal projection of the vector PQ onto the n-u dimensional hyperplane as described above, and it ensures that regardless of the location of the point P in the model surface, the Q-surface passes through the point Q. This construction has the advantage of

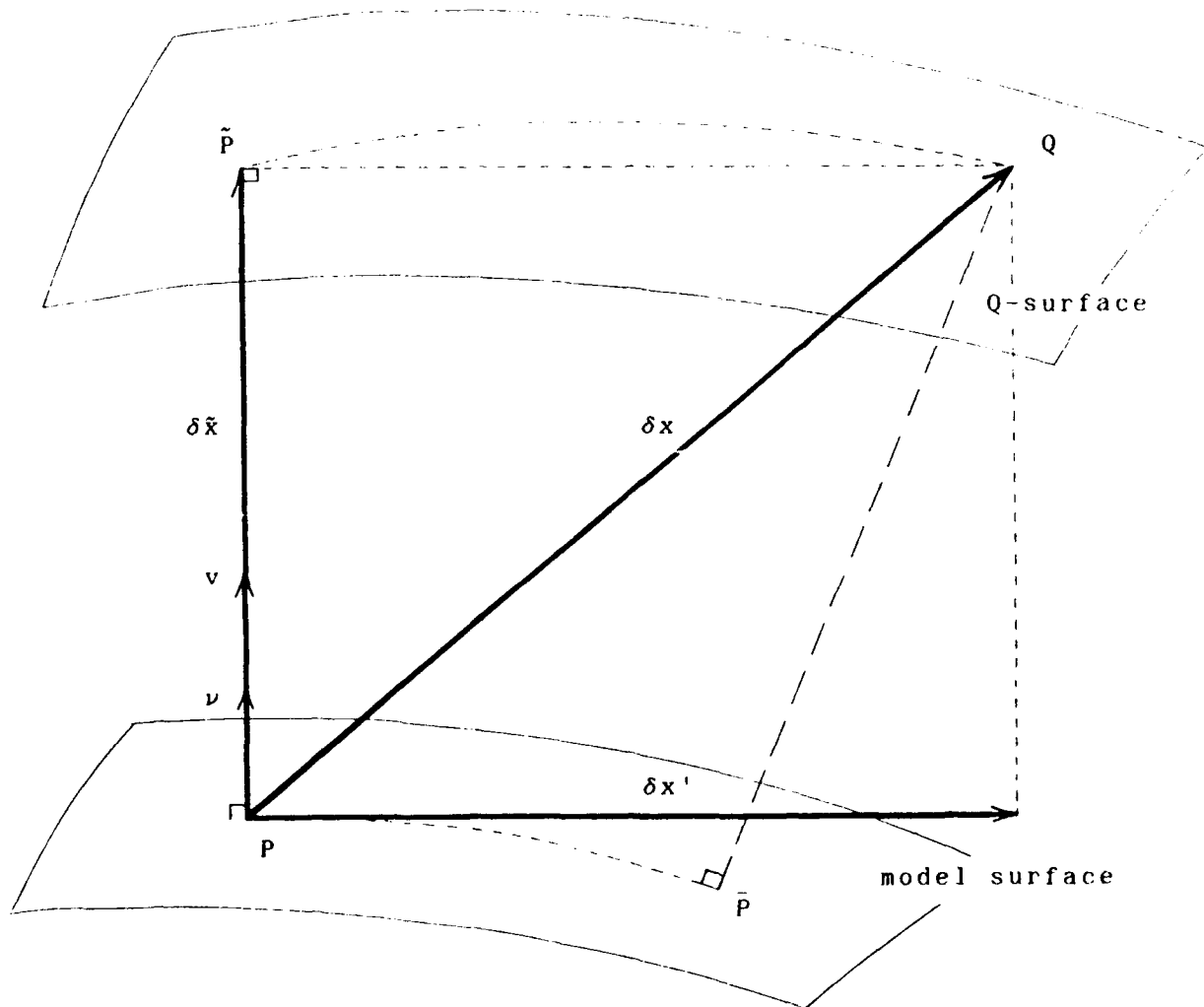
utilizing a set of gradients N_r^L (represented by the vectors v), which can be easily expressed from the functional form of the model surface (as obtained in the first step), and of projecting Q orthogonally onto the hyperplane generated by these gradients, which is a linear operation.

In analogy to the definition of the (new) model-surface coordinates x^α , in the third step we adopt the first u of the n space coordinates x^r as the Q -surface coordinates, denoted \tilde{x}^α for easy reference, and express their variations in terms of variations of the model-surface coordinates x^α . Since the spatial positions of points in the Q -surface are linked to the sets of gradients N_r^L at the corresponding points in the model surface, the variations in \tilde{x}^α entail the differentiation of N_r^L with respect to x^α . This differentiation (a part of the first step) is facilitated by the relative simplicity of the functional form (7). The mapping of the variations of x^α into the variations of \tilde{x}^α can be expressed by the Taylor series, similar to a coordinate transformation in one and the same surface.

Such a series can, in turn, be inverted analytically, and the inverted series can be used to describe the variations of x^α in terms of the variations of \tilde{x}^α . The important characteristic of the process resulting in the original and the inverted series is that, again, only linear operations are involved. Since both the point \tilde{P} (generated from the initial point P) and the point Q are known in all n coordinates, and since both lie on the Q -surface, their coordinate differences $\Delta\tilde{x}^\alpha$ are known. In using the inverted series, one can then determine the unknown model-surface coordinate differences Δx^α between the points P and \tilde{P} .

After the determination of the coordinates x^α , the remaining coordinates, x^L , follow from (6b). Thus, insofar as the observational-space coordinates are concerned, the geometrical problem of determining \tilde{P} is solved. In the adjustment context, this represents the solution of adjusted observations but not adjusted parameters. As the fourth and last step, the related geometrical task, i.e., the determination of the original model-surface coordinates of \tilde{P} , can be accomplished via the initial inverse equation (6a). This relation, like others encountered above, is expressible by the Taylor series expansion from the initial point P , and can thus be resolved by means of linear operations.

GENERATION OF A TWO-DIMENSIONAL Q-SURFACE
FROM A TWO-DIMENSIONAL MODEL SURFACE



Point P lies in a two-dimensional model surface

\tilde{P} corresponds to P; similarly, other points \tilde{P} would be constructed
from other points P

Fig. 2

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4. DEVELOPMENT OF THE FUNCTIONAL-FORM APPROACH IN FOUR STEPS

4.1 First-Step Derivation

In (4), the model surface is given in the Gauss form via $x^r = x^r(u^\beta)$. This form is known, as are the partial derivatives listed here to the third order:

$$\partial x^r / \partial u^\alpha = A_\alpha^r, \quad \partial^2 x^r / \partial u^\alpha \partial u^\beta = \Omega_{\alpha\beta}^r, \quad \partial^3 x^r / \partial u^\alpha \partial u^\beta \partial u^\gamma = \Phi_{\alpha\beta\gamma}^r. \quad (9a,b,c)$$

Each of these sets is partitioned into two subsets:

$$A_\alpha^r = \{A_\alpha^\rho, A_\alpha^R\}, \quad \Omega_{\alpha\beta}^r = \{\Omega_{\alpha\beta}^\rho, \Omega_{\alpha\beta}^R\}, \quad \Phi_{\alpha\beta\gamma}^r = \{\Phi_{\alpha\beta\gamma}^\rho, \Phi_{\alpha\beta\gamma}^R\}, \quad (10a,b,c)$$

where, in agreement with the previous convention, the lower-case Greek indices range from 1 to u , the upper-case Roman indices range from $u+1$ to n , or, equivalently, from 1 to $n-u$, and the lower-case Roman indices range from 1 to n .

In consulting (6b)-(8), we define (space) scalar functions of position N^L as

$$N^L = x^L - f^L(x^\alpha) = x^L - x^L(u^\beta(x^\alpha)),$$

and stipulate that along the model surface they take on the constant value of zero. Their gradients in the coordinate system $\{x^r\}$ follow as

$$N_r^L = \partial N^L / \partial x^r = \{\partial N^L / \partial x^\rho, \partial N^L / \partial x^R\} = \{-\partial x^L / \partial x^\rho, \delta_R^L\},$$

which we write in the form

$$N_\rho^L = \partial N^L / \partial x^\rho = -\partial x^L / \partial x^\rho, \quad (11a)$$

$$N_R^L = \partial N^L / \partial x^R = \delta_R^L; \quad (11b)$$

we keep in mind that the quantities x^L in (11a) and the equation above it represent f^L , functions of the first u space coordinates as introduced in (6b).

The nonzero second- and third-order partial derivatives are

$$N_{\rho\mu}^L = \partial^2 N^L / \partial x^\rho \partial x^\mu = -\partial^2 x^L / \partial x^\rho \partial x^\mu, \quad (12a)$$

$$N_{\rho\mu\tau}^L = \partial^3 N^L / \partial x^\rho \partial x^\mu \partial x^\tau = -\partial^3 x^L / \partial x^\rho \partial x^\mu \partial x^\tau. \quad (12b)$$

If we adopt $\{x^\alpha\}$ as a new set of model-surface coordinates, the Gauss form of the surface can be written as $x^r = h^r(x^\alpha)$, representing $\{x^\rho, x^R\} = \{x^\rho, f^R(x^\alpha)\}$. The new partial derivatives (listed to the third order) become

$$\partial x^r / \partial x^\alpha = \{\partial x^\rho / \partial x^\alpha, \partial x^R / \partial x^\alpha\} = \{\delta_\alpha^\rho, -N_\alpha^R\}, \quad (13a)$$

$$\partial^2 x^r / \partial x^\alpha \partial x^\beta = \{\partial^2 x^\rho / \partial x^\alpha \partial x^\beta, \partial^2 x^R / \partial x^\alpha \partial x^\beta\} = \{0, -N_{\alpha\beta}^R\}, \quad (13b)$$

$$\partial^3 x^r / \partial x^\alpha \partial x^\beta \partial x^\gamma = \{\partial^3 x^\rho / \partial x^\alpha \partial x^\beta \partial x^\gamma, \partial^3 x^R / \partial x^\alpha \partial x^\beta \partial x^\gamma\} = \{0, -N_{\alpha\beta\gamma}^R\}. \quad (13c)$$

It should be mentioned that these (as well as the previous) partial derivatives are considered at the point P of the model surface. This understanding applies also for the subsequent paragraphs.

We now introduce the following notation for the (unknown) partial derivatives of the original model-surface coordinates with respect to the new model surface coordinates:

$$\partial u^\alpha / \partial x^\beta = R_\beta^\alpha, \quad \partial^2 u^\alpha / \partial x^\beta \partial x^\gamma = A_{\beta\gamma}^\alpha, \quad \partial^3 u^\alpha / \partial x^\beta \partial x^\gamma \partial x^\delta = \Theta_{\beta\gamma\delta}^\alpha. \quad (14a, b, c)$$

Next, we use the space-surface differential relation

$$\partial x^r / \partial x^\kappa = (\partial x^r / \partial u^\lambda) (\partial u^\lambda / \partial x^\kappa), \quad (15)$$

where the left-hand side is akin to (9a). Due to (13a), (9a) together with (10a), and (14a), equation (15) reads

$$\{\delta_\kappa^\rho, -N_\kappa^R\} = \{A_\lambda^\rho, A_\lambda^R\} R_\kappa^\lambda.$$

After changing the free indices ρ and R , one then obtains

$$A_\lambda^\alpha R_\kappa^\lambda = \delta_\kappa^\alpha, \quad (16a)$$

$$N_\kappa^L = -A_\lambda^L R_\kappa^\lambda. \quad (16b)$$

In matrix notation, (16a) means that

$$[R_\kappa^\lambda] = [A_\lambda^\alpha]^{-1}, \quad (16a')$$

where the indices are now meaningless.

Next, we differentiate (15) further:

$$\partial^2 x^r / \partial x^\kappa \partial x^\tau = \partial / \partial x^\tau (\partial x^r / \partial x^\kappa) = \partial / \partial x^\tau [(\partial x^r / \partial u^\beta) (\partial u^\beta / \partial x^\kappa)].$$

The right-hand side of this equation is composed of two terms, the first of which is obtained with the aid of $\partial/\partial x^\tau (\partial x^r/\partial u^\beta) = (\partial^2 x^r/\partial u^\beta \partial u^\gamma) (\partial u^\gamma/\partial x^\tau)$. Thus, we have

$$\begin{aligned} \partial^2 x^r / \partial x^\kappa \partial x^\tau = & (\partial^2 x^r / \partial u^\beta \partial u^\gamma) (\partial u^\beta / \partial x^\kappa) (\partial u^\gamma / \partial x^\tau) \\ & + (\partial x^r / \partial u^\beta) (\partial^2 u^\beta / \partial x^\kappa \partial x^\tau) . \end{aligned} \quad (17)$$

According to (13b), the left-hand side above is $\{0, -N_{\kappa\tau}^R\}$; according to (9b) together with (10b), and (14a), the factors in the first term on the right-hand side are $\Omega_{\beta\gamma}^r \equiv \{\Omega_{\beta\gamma}^\rho, \Omega_{\beta\gamma}^R\}$, R_κ^β , and R_τ^γ ; and according to (9a) together with (10a), and (14b), the factors in the second term on the right-hand side are $A_\beta^r \equiv \{A_\beta^\rho, A_\beta^R\}$ and $\Lambda_{\kappa\tau}^\beta$. Equation (17) is seen to represent two equalities. Upon the contraction with R_ρ^λ and the use of (16a), the first equality yields

$$\Lambda_{\kappa\tau}^\lambda = -R_\mu^\lambda \Omega_{\beta\gamma}^\mu R_\kappa^\beta R_\tau^\gamma . \quad (18a)$$

With this result as well as (10b), the second equality yields

$$N_{\kappa\tau}^L = -(N_\mu^L \Omega_{\beta\gamma}^\mu + \Omega_{\beta\gamma}^L) R_\kappa^\beta R_\tau^\gamma . \quad (18b)$$

The changes in indices (two in dummy indices, one in a free index) which have entered these two formulas need no elaboration.

Similar to the differentiation of (15) which has lead to (17) and finally to (18a,b), we now differentiate (17) with respect to x^ω . Straightforward algebraic manipulations, where advantage is taken of the fact that the partial derivatives commute, again result in two equalities. The first reads

$$\Theta_{\kappa\tau\omega}^\lambda = -R_\mu^\lambda [\Phi_{\beta\gamma\delta}^\mu R_\kappa^\beta R_\tau^\gamma R_\omega^\delta + \Omega_{\beta\gamma}^\mu (R_\kappa^\beta \Lambda_{\tau\omega}^\gamma + R_\tau^\beta \Lambda_{\omega\kappa}^\gamma + R_\omega^\beta \Lambda_{\kappa\tau}^\gamma)] , \quad (19a)$$

and the second reads

$$\begin{aligned} N_{\kappa\tau\omega}^L = & -[(N_\mu^L \Phi_{\beta\gamma\delta}^\mu + \Phi_{\beta\gamma\delta}^L) R_\kappa^\beta R_\tau^\gamma R_\omega^\delta \\ & + (N_\mu^L \Omega_{\beta\gamma}^\mu + \Omega_{\beta\gamma}^L) (R_\kappa^\beta \Lambda_{\tau\omega}^\gamma + R_\tau^\beta \Lambda_{\omega\kappa}^\gamma + R_\omega^\beta \Lambda_{\kappa\tau}^\gamma)] . \end{aligned} \quad (19b)$$

In passing from (19a) to (19b), $R_\mu^\lambda \Omega_{\beta\gamma}^\mu$ has been replaced by $N_\mu^L \Omega_{\beta\gamma}^\mu + \Omega_{\beta\gamma}^L$, the same as when passing from (18a) to (18b), and $R_\mu^\lambda \Phi_{\beta\gamma\delta}^\mu$ has been replaced by $N_\mu^L \Phi_{\beta\gamma\delta}^\mu + \Phi_{\beta\gamma\delta}^L$.

In summary, the first-, second-, and third order partial derivatives of the original model-surface coordinates u^α with respect to the new model-surface

coordinates x^α as outlined in (14a,b,c) are given by (16a) or (16a'), (18a), and (19a), respectively. And the first-, second-, and third order partial derivatives of the scalar functions N^L with respect to the new model-surface coordinates x^α , initially presented in (11a) and (12a,b), are given by (16b), (18b), and (19b), respectively.

4.2 Q-Surface Determination

The determination of the Q-surface will now be described in detail. Since any chosen point of the model surface generates a unique corresponding point in the Q-surface, we need only to express a typical vector $\delta\tilde{x}$, such as illustrated in Fig. 2 and 3. The contravariant and covariant components of this vector are denoted $\delta\tilde{x}^r$ and $\delta\tilde{x}_s$, respectively, linked together in a familiar relation:

$$\delta\tilde{x}^r = g^{rs} \delta\tilde{x}_s, \quad (20)$$

where g^{rs} is the associated metric tensor (here constant). The contravariant components δx^r of the vector δx (illustrated in Fig. 1-3) represent the basic known quantities. The n -u gradients N_r^L , in Fig. 2 and 3 represented by the vectors v , comprise another set of known quantities associated with P. Since $\delta\tilde{x}$ is orthogonal to the model surface, it must be expressible as a linear combination of the vectors v . In covariant components, we thus have

$$\delta\tilde{x}_s = N_s^M c_M, \quad (21)$$

where c_M are n -u coefficients; the index M (or another upper-case Roman index) attributed to c acts only in a "countable" role, similar to that explained below equation (8) in conjunction with the functions N . Thus, c_M is not a covariant tensor, but is contracted with N_s^M in accordance with the summation convention.

On the other hand, δx^r is stipulated to be a vector tangent to the model surface at P; it is thus orthogonal to the vectors v . This vector is constrained by the requirement that when it is added vectorially to $\delta\tilde{x}$, the result is δx (see also Fig. 2 and 3). In contravariant components (and similarly in covariant components), one then has the tensor equation at P:

$$\delta x^r = \delta x^r + \delta\tilde{x}^r, \quad (22)$$

where $\delta x'^r$ and $\delta \tilde{x}^r$ are unknown so far. The above tangential property is reflected in

$$N_r^L \delta x'^r = N_r^L (\delta x^r - \delta \tilde{x}^r) = 0, \quad (23)$$

where the "0" on the right-hand side represents $n-u$ zero elements. At this stage we use (20) and (21) in expressing $\delta \tilde{x}^r$ in terms of the unknown coefficients and the known gradients, so that (23) becomes

$$N_r^L g^{rs} N_s^M c_M = N_r^L \delta x^r. \quad (24)$$

If the gradients of N for each L (or M) are considered as column-vectors of n elements grouped into the matrix R^* of dimensions $n \times (n-u)$, the components g^{rs} are grouped into the positive-definite (symmetric) matrix g of dimensions $n \times n$, the components δx^r are grouped into the column vector δx of dimensions $n \times 1$, and the coefficients symbolized by c_M are grouped into the column-vector c of dimensions $(n-u) \times 1$, equation (24) reads

$$(R^{*T} g R^*) c = R^{*T} \delta x. \quad (24')$$

The transformation from (24) to (24') does not reveal the usual correspondence between tensor contractions and matrix multiplications as we would expect it if L and M were "regular" tensor indices, since in such cases we would treat the contravariant (upper) index as the first, and the covariant (lower) index as the second. However, in their "countable" role, L and M are written in the upper position in N_r^L , etc., for convenience, and could as well have been utilized in the form N_{rL} , etc. In fact, in view of matrix transcriptions (which are completely unnecessary), such an alternative form corresponds to the above construction of the matrix R^* , and results in (24') by virtue of the summation convention used in (24).

Next, an array quantity B^{LM} is introduced, containing $(n-u) \times (n-u)$ scalar invariants associated with P , according to the definition

$$B^{LM} = N_r^L g^{rs} N_s^M. \quad (25)$$

In matrix form, this can be transcribed as

$$B = R^{*T} g R^*. \quad (25')$$

where B is a positive-definite (symmetric) matrix of dimensions $(n-u) \times (n-u)$, due to the fact that g is positive-definite (symmetric) and that R^* has the full column rank $n-u$ (it contains $n-u$ independent gradient vectors generating an $n-u$ dimensional hyperplane). We now consider an array quantity Q_{KL} defined through the Kronecker delta such that

$$Q_{KL} B^{LM} = \delta_K^M, \quad (26)$$

which, in matrix notation, would correspond to

$$QB = I, \quad Q = B^{-1} = (R^{*T} g R^*)^{-1}. \quad (26')$$

In contracting (24) with Q_{KL} and recalling (25) and (26), we obtain

$$c_K = Q_{KL} N_r^L \delta x^r, \quad (27)$$

where $\delta_K^M c_M = c_K$ has been utilized. In matrix notation this would read

$$c = Q R^{*T} \delta x = (R^{*T} g R^*)^{-1} R^{*T} \delta x. \quad (27')$$

Finally, with the aid of (21) and (27), the contravariant vector $\delta \tilde{x}^r$ from equation (20) is expressed as

$$\delta \tilde{x}^r = g^{rs} N_s^K c_K = g^{rs} N_s^K Q_{KL} N_m^L \delta x^m, \quad (28)$$

which, in matrix notation, would be

$$\delta \tilde{x} = g R^* c = g R^* (R^{*T} g R^*)^{-1} R^{*T} \delta x, \quad (28')$$

where the n components of $\delta \tilde{x}^r$ have been grouped into the column-vector $\delta \tilde{x}$.

As a matter of interest, we remark that due to the general relation

$$k^r = g^{rs} k_s, \quad k_s = g_{sr} k^r,$$

the set of (covariant) gradient vectors could have been transformed by $g^{rs} N_s^L$ into a set of contravariant vectors, which could have then been grouped into the matrix R of dimensions $n \times (n-u)$. This amounts to writing

$$R = g R^*, \quad R^* = g^* R,$$

upon the realization that $g = (g^*)^{-1}$, where g^* groups the components of g_{sr} .

Accordingly, equations (27') and (28') could have been formulated in terms of R :

$$c = (R^T g^* R)^{-1} R^T g^* \delta x ,$$

$$\delta \tilde{x} = R (R^T g^* R)^{-1} R^T g^* \delta x ,$$

which have a form akin to that for the parametric corrections and the observational corrections, respectively, in the parametric least-squares adjustment, with R corresponding to the design matrix, g^* corresponding to the weight matrix, and δx corresponding to the vector of (reduced) observations. However, the original formulation transcribed as (27') and (28') is far more advantageous in the present context, since the initially known quantities are the gradient sets N_r^L forming R^* and the observational variance-covariances forming g .

Clearly, the matrix transcriptions and the adjustment analogies have been incidental to the present development, and could have been left out altogether. However, their presentation may be useful for their instructive value, especially in considering that the adjustment topics have been traditionally exposed in matrix notation. In closing, we recapitulate the outcome related to the Q -surface determination in a concise-manner:

$$\delta \tilde{x}^r = g^{rs} N_s^K c_K , \quad (29a)$$

where

$$c_K = Q_{KL} N_m^L \delta x^m , \quad (29b)$$

and where

$$Q_{KL} B^{LM} = \delta_K^M , \quad B^{LM} = N_r^L g^{rs} N_s^M . \quad (29c)$$

4.3 Third and Fourth Steps

In its geometric analogy, nonlinear parametric adjustment has been seen to correspond to the task of drawing a geodesic in an n -dimensional observational space orthogonally to a u -dimensional model surface. The relative simplicity of this task stems from the fundamental property that the observational-space metric tensor is constant. Accordingly, the observational-space coordinate system, symbolized by $\{x^r\}$, can be thought of as oblique Cartesian, and a coordinate set x^r of a given point can be thought of as a contravariant position-

vector ρ^r . This interpretation allows us to write what may appear as a mixture of vector components (here δx^r) and coordinates (here x^r):

$$\delta x^r = x^r(Q) - x^r(P) \quad (30)$$

where the letters in parentheses denote the points in question. Before commenting further, we introduce the notational conventions as follows.

(i) The point Q, corresponding to the outcome of observations, is considered fixed, and its coordinate sets are henceforth attributed the subscript Q instead of being identified by "(Q)".

(ii) The point P is considered to be a variable point of the model surface, and its coordinate sets are henceforth attributed no identification; thus, instead of writing $x^r(P)$, we will write simply x^r .

(iii) The point \tilde{P} of the Q-surface, corresponding to the point P of the model surface, could have been identified by the coordinate set written as $x^r(\tilde{P})$, similar to the original notation $x^r(P)$ seen in (30). However, due to the letters in parentheses being dropped, we replace "x" by " \tilde{x} " for any point of the Q-surface; thus, $x^r(P)$ and $x^r(\tilde{P})$ are replaced by x^r and \tilde{x}^r , respectively. This convention applies also for subsets of the first u or the last n-u coordinates, such as in x^α and \tilde{x}^α , or x^L and \tilde{x}^L . When referring to the fixed point Q (rather than to the variable point P or its counterpart \tilde{P}), we use the subscript Q as stipulated in item (i), i.e., we write \tilde{x}_Q^r and, eventually, \tilde{x}_Q^α or \tilde{x}_Q^L .

With the above conventions, equation (30) is written as

$$\delta x^r = \tilde{x}_Q^r - x^r \quad (31)$$

If \tilde{x}_Q^r and x^r are interpreted as contravariant position vectors belonging to P, then (31) represents a tensor equation at P. In fact, due to the character of $\{x^r\}$ alluded to above (oblique Cartesian coordinates), the coordinate set x^r can be identified with the contravariant position-vector associated with P. Although \tilde{x}_Q^r is identified with the contravariant position vector associated with Q, the character of $\{x^r\}$ allows this position-vector to be freely parallel transported to P or any other location; the "free" parallel transport implies that no change in the components has taken place. Similarly, we have

$$\delta \tilde{x}^r = \tilde{x}^r - x^r \quad (32)$$

which can again be interpreted as a tensor equation at P. The geometrical objects representing the contravariant vectors δx^r and $\delta \tilde{x}^r$ are δx and $\delta \tilde{x}$, referred to simply as vectors, which are illustrated in Fig. 2 and 3. In the following, we will consider only a subset of (32) encompassing the first u out of n components. The pertinent relation, namely

$$\delta \tilde{x}^\alpha = \tilde{x}^\alpha - x^\alpha, \quad (32')$$

is not a tensor equation, but merely an equality for the selected components. This, however, does not detract from its usefulness in the present development.

We use (32') in the form

$$\tilde{x}^\alpha = x^\alpha + \delta \tilde{x}^\alpha, \quad (33)$$

from which we can deduce that \tilde{x}^α is a function of x^α . In fact, from (28) or (29a), $\delta \tilde{x}^\alpha$ follows from $\delta \tilde{x}^r$ upon replacing g^{rs} by $g^{\alpha s}$:

$$\delta \tilde{x}^\alpha = g^{\alpha s} N_{s Q_{KL}}^K N_m^L \delta x^m. \quad (34)$$

First of all, g^{rs} is constant; this property affects $g^{\alpha s}$ above, as well as Q_{KL} via B^{LM} (see equation 29c). From (11a,b) it is apparent that N_r^L is a function of x^α . Finally, δx^m is written as

$$\delta x^m \equiv \{\delta x^\mu, \delta x^M\}, \quad (35)$$

where, due to (31), one has

$$\delta x^\mu = \tilde{x}_Q^\mu - x^\mu, \quad \delta x^M = \tilde{x}_Q^M - x^M. \quad (35')$$

Here \tilde{x}_Q^μ and \tilde{x}_Q^M are constant, while x^M is a function of x^μ as was already stated in (6b), in conjunction with the Monge form of the model surface. It then follows that $\delta \tilde{x}^\alpha$, and therefore \tilde{x}^α , are functions of x^α (see equations 34 and 33). A similar statement can also be made with respect to the "full" version of (33), corresponding to equation (32).

We are now in a position to present the concept of the determination of the least-squares point \bar{P} based on the role played by the Q-surface. This point is regarded as the location of the variable point P which entails $\tilde{x}^\alpha = \tilde{x}_Q^\alpha$, i.e., for which the Q-surface points \tilde{P} and Q coincide.

(a) The crucial element of the least-squares resolution is the set of u coordinates x^α of the variable point P when the latter coincides with \bar{P} .

(The remaining $n-u$ space coordinates, x^L , can be found via the Monge form of the model surface as presented in equation 6b, and the u model-surface coordinates u^α for this point can be found via equation 6a.)

(b) The set x^α associated with the variable point P can be obtained from a set of u variables if the functional relationship between the two sets is known. (If this relationship is formulated through sets of partial derivatives, the set x^α can be expressed by the Taylor-series expansion; such a formulation is sufficient to consider the relationship as known.)

(c) The just-mentioned u variables are represented here by the coordinate set \tilde{x}^α . To elaborate, we first state that the sets x^r and $\delta\tilde{x}^r$ are known functions of x^α . Accordingly, due to $\tilde{x}^r = x^r + \delta\tilde{x}^r$, we can also state that the set \tilde{x}^r and any of its subsets are known functions of x^α . A simple and natural manner, then, in which to choose a suitable set of u variables consists in adopting the first u out of n relations represented by this tensor equation, namely $\tilde{x}^\alpha = x^\alpha + \delta\tilde{x}^\alpha$, which has appeared as (33).

(d) By virtue of the known functional relationship between the sets x^α and \tilde{x}^α associated with P and \tilde{P} , respectively, we can express the coordinate differences $\Delta\tilde{x}^\alpha$ in terms of Δx^α and vice-versa. Since this known relationship reflects the fact that the vector $\tilde{P}\tilde{P}$ is orthogonal to the model surface, any new pair of points P and \tilde{P} (found upon applying the coordinate differences to a previous pair) will preserve this quality.

(e) We next consider one position of P as known, but keep the notation unaffected by this designation. Such an "initial" point is given by the model-surface coordinates u^α , from which the observational-space coordinates x^r follow by (4). The sets δx^r , $\delta\tilde{x}^\alpha$, and \tilde{x}^α associated with this point are then known from (31), (34), and (33), respectively. Since \tilde{x}_Q^α is known, so is now $\Delta\tilde{x}^\alpha \equiv \tilde{x}_Q^\alpha - \tilde{x}^\alpha$. This leads to Δx^α and thus to the model-surface coordinates of a new point P , whose corresponding point \tilde{P} is Q (due to the definition of $\Delta\tilde{x}^\alpha$). Accordingly, the new point P is the desired least-squares point \bar{P} .

(f) Since the (new) model-surface coordinates have been defined as $\{x^\alpha\}$, and similarly the Q -surface coordinates can be defined as $\{\tilde{x}^\alpha\}$, the procedure described in items (d) and (e) transforms coordinates between two surfaces. This approach is based on the known functional relationship between the two

kinds of coordinates, dictated by the known correspondence between points in one and the other surface (points "P" and points " \tilde{P} "). We comment that such a procedure is akin to the transformation of coordinates in one and the same surface, based on a known functional relationship between the coordinate sets.

The implementation of the above concept proceeds along the following lines. Since the observables correspond to the observational-space coordinates $\{x^r\}$ and the parameters correspond to the model-surface coordinates $\{u^\alpha\}$, the adjustment model is interpreted in the geometrical context as $x^r = x^r(u^\alpha)$, appearing in (4). The known coordinates u^α of the initial point P then lead to x^r . The first-, second-, third-, ... order partial derivatives of $x^r(u^\alpha)$ with respect to the model-surface coordinates, evaluated at P, compose the arrays A_α^r , $\Omega_{\alpha\beta}^r$, $\Phi_{\alpha\beta\gamma}^r$, The design matrix A of the standard adjustment setup corresponds to the "design tensor" A_α^r . The actual observations are interpreted to correspond to \tilde{x}_Q^r , and the variance-covariance matrix of observations is interpreted to correspond to g^{rs} , the (space) associated metric tensor; the latter, just as the metric tensor g_{rs} , is stipulated to be constant. The known \tilde{x}_Q^r and x^r give δx^r by (31), which then leads to $\delta \tilde{x}^\alpha$ according to (34).

Since a close-form relationship between \tilde{x}^α and x^α via (33) and (34) would be intractable and nearly impossible to establish, we relate the two sets through their partial derivatives:

$$\tilde{A}_\beta^\alpha \equiv \partial \tilde{x}^\alpha / \partial x^\beta = \delta_\beta^\alpha + \partial \delta \tilde{x}^\alpha / \partial x^\beta, \quad (36)$$

$$\tilde{\Omega}_{\beta\gamma}^\alpha \equiv \partial^2 \tilde{x}^\alpha / \partial x^\beta \partial x^\gamma = \partial^2 \delta \tilde{x}^\alpha / \partial x^\beta \partial x^\gamma, \quad (37)$$

etc., which are based on (33). These arrays can be expressed from (34), where all the quantities on the right-hand side except $g^{\alpha\beta}$ (constant) are functions of x^α , to be evaluated with the coordinates of P. To formulate the set of coordinate differences $\Delta \tilde{x}^\alpha$ defined in item (e) above, we first write

$$\delta x'^r = \delta x^r - \delta \tilde{x}^r = \tilde{x}_Q^r - \tilde{x}^r,$$

where the first equality is (22), and the second equality is the consequence of (31) and (32). In view of the character of the coordinate system $\{x^r\}$, it is not surprising that $\delta x'^r$, a (space) contravariant vector at P, is expressible in terms of coordinate differences. Upon considering the first u out of n components in this relation, it follows that

$$\Delta \tilde{x}^\alpha \equiv \tilde{x}_Q^\alpha - x^\alpha = \delta x^\alpha - \delta \tilde{x}^\alpha . \quad (38)$$

We remark that this equation, together with the first equation of (35'), yields

$$\partial \Delta \tilde{x}^\alpha / \partial x^\beta = -(\delta_\beta^\alpha + \partial \delta \tilde{x}^\alpha / \partial x^\beta) , \quad (38')$$

which is $-\tilde{A}_\beta^\alpha$. The left-hand side of (38') is one of several expressions encountered in an initial formulation of $\tilde{\Omega}_{\beta\gamma}^\alpha$.

Equations (36), (37), ... would allow us to express $\Delta \tilde{x}^\alpha$ from Δx^α via the Taylor series. However, here we are seeking Δx^α based on $\Delta \tilde{x}^\alpha$. The reversed partial derivatives, needed for a reversed series, are denoted as

$$\partial x^\alpha / \partial \tilde{x}^\beta = \tilde{R}_\beta^\alpha , \quad \partial^2 x^\alpha / \partial \tilde{x}^\beta \partial \tilde{x}^\gamma = \tilde{\Lambda}_{\beta\gamma}^\alpha , \dots$$

They can be obtained from \tilde{A}_β^α , $\tilde{\Omega}_{\beta\gamma}^\alpha$, ... upon using the approach that resulted in R_β^α , $\Lambda_{\beta\gamma}^\alpha$, ... in (16a), (18a), ... , based on A_β^α , $\Omega_{\beta\gamma}^\alpha$, That is to say, equations (16a), (18a), ... can be re-used with all the quantities attributed the symbol "~". Thus, the array \tilde{R}_β^α is determined from

$$\tilde{A}_\lambda^\alpha \tilde{R}_\kappa^\lambda = \delta_\kappa^\alpha ; \quad (39)$$

in matrix notation this implies that

$$[\tilde{R}_\kappa^\lambda] = [\tilde{A}_\lambda^\alpha]^{-1} , \quad (39')$$

where the indices are now meaningless. Similarly, the array $\tilde{\Lambda}_{\beta\gamma}^\alpha$ is given by

$$\tilde{\Lambda}_{\beta\gamma}^\alpha = -\tilde{R}_\mu^\alpha \tilde{\Omega}_{\mu\eta}^\mu \tilde{R}_\eta^\gamma \tilde{R}_\beta^\tau . \quad (40)$$

The above equations may appear simple, but they are greatly complicated by the complexity of \tilde{A}_β^α , $\tilde{\Omega}_{\beta\gamma}^\alpha$, For example, we can show that

$$\tilde{A}_\beta^\alpha = \delta_\beta^\alpha + T^{\alpha\mu} E_{\mu\beta} + G_L^{\alpha} U_\beta^L , \quad (41)$$

where

$$T^{\alpha\mu} = g^{\alpha\mu} - G_K^{\alpha} P^{\mu K} , \quad E_{\mu\beta} = c_K N_{\mu\beta}^K ,$$

$$G_L^\alpha = P^{\alpha K} Q_{KL} , \quad U_\beta^L = N_{\beta\mu}^L \Delta \tilde{x}^\mu ;$$

$$P^{\alpha K} = g^{\alpha s} N_s^K - g^{\alpha\tau} N_\tau^K + g^{\alpha K} , \quad c_K = Q_{KL} W^L ,$$

$$W^L = N_m^L \delta x^m = N_\mu^L \delta x^\mu + \delta x^L ;$$

furthermore,

$$B^{MN}Q_{NK} = \delta_K^M, \quad \text{or} \quad [Q_{NK}] = [B^{MN}]^{-1},$$

where

$$B^{KM} = N_r^K g^{rs} N_s^M = N_\gamma^K g^{\gamma\delta} N_\delta^M + g^{K\delta} N_\delta^M + N_\delta^K g^{\delta M} + g^{KM},$$

in which we have used (11b). As is illustrated above, also the quantities N_μ^L , $N_{\mu\eta}^L$, ... are involved in the formation of \tilde{A}_β^α , $\tilde{\Omega}_{\beta\gamma}^\alpha$, Fortunately, these quantities have been found in conjunction with the development of R_β^α , $\Lambda_{\beta\gamma}^\alpha$, ... (see equations 16b, 18b, ...). The coordinate differences $\Delta\tilde{x}^\mu$ in the formula for U_β^L are those featured in (38).

The derivation leading to (41) will now be outlined. We begin with (34), which is transcribed as

$$\delta\tilde{x}^\alpha = P^{\alpha K} Q_{KL} W^L = G_L^\alpha W^L.$$

Accordingly, we have

$$\partial\delta\tilde{x}^\alpha/\partial x^\beta = (\partial P^{\alpha K}/\partial x^\beta) Q_{KL} W^L + P^{\alpha K} [(\partial Q_{KL}/\partial x^\beta) W^L + Q_{KL} (\partial W^L/\partial x^\beta)],$$

where

$$\partial P^{\alpha K}/\partial x^\beta = g^{\alpha\tau} N_{\tau\beta}^K,$$

$$\partial W^L/\partial x^\beta = N_{\mu\beta}^L \delta x^\mu + N_\mu^L (\partial\delta x^\mu/\partial x^\beta) + \partial\delta x^L/\partial x^\beta = N_{\mu\beta}^L \delta x^\mu;$$

the last outcome is due to the cancellation stemming from $\partial\delta x^\mu/\partial x^\beta = -\delta_\beta^\mu$ and $\partial\delta x^L/\partial x^\beta = -\partial x^L/\partial x^\beta = N_\beta^L$. The expression for $\partial Q_{KL}/\partial x^\beta$ follows from the differentiation of the form $B^{MK}Q_{KL} = \delta_L^M$, where this equation itself, as well as the symmetry of B^{MK} and hence of Q_{KL} , are also utilized. The result is

$$\partial Q_{KL}/\partial x^\beta = -(G_K^\mu Q_{LS} + G_L^\mu Q_{KS}) N_{\mu\beta}^S.$$

Upon using the previously introduced notation, we obtain

$$\partial\delta\tilde{x}^\alpha/\partial x^\beta = T^{\alpha\mu} E_{\mu\beta} + G_L^\alpha U_\beta^L,$$

and, due to (36), verify (41).

The principles that have led to (41) can be further expanded to yield $\tilde{\Omega}_{\beta\gamma}^\alpha$. We list the final results of this development in the form $\tilde{\Omega}_{\beta\gamma}^\alpha \delta x^\beta \delta x^\gamma$ as needed for the contraction

$$\tilde{\Lambda}_{\beta\gamma}^{\alpha} \Delta \tilde{x}^{\beta} \Delta \tilde{x}^{\gamma} = -\tilde{R}_{\mu}^{\alpha} \tilde{\Omega}_{\beta\gamma}^{\mu} \tilde{R}_{\kappa}^{\beta} \tilde{R}_{\tau}^{\gamma} \Delta \tilde{x}^{\kappa} \Delta \tilde{x}^{\tau} = -\tilde{R}_{\mu}^{\alpha} \tilde{\Omega}_{\beta\gamma}^{\mu} dx^{\beta} dx^{\gamma} ,$$

where

$$dx^{\beta} = \tilde{R}_{\omega}^{\beta} \Delta \tilde{x}^{\omega} .$$

In a form suitable for programming, where vectors such as dx^{α} first contract higher-dimensional arrays in order to lower the dimensionality, we have

$$\tilde{\Omega}_{\beta\gamma}^{\mu} dx^{\beta} dx^{\gamma} = T^{\mu\phi} p_{\phi} + G_K^{\mu} q^K , \quad (42)$$

where

$$p_{\phi} = c_K N_{\phi\alpha\beta}^K dx^{\alpha} dx^{\beta} + 2 d_K N_{\phi\alpha}^K dx^{\alpha} ,$$

$$d_K = Q_{KL} U_{\beta}^L dx^{\beta} - E_{\phi\beta} dx^{\beta} G_K^{\phi} ;$$

$$q^K = N_{\mu\alpha\beta}^K dx^{\alpha} dx^{\beta} \Delta \tilde{x}^{\mu} - N_{\alpha\beta}^K dx^{\alpha} dx^{\beta} - 2 N_{\mu\alpha}^K dx^{\alpha} (\partial \delta \tilde{x}^{\mu} / \partial x^{\beta}) dx^{\beta} ,$$

where $\partial \delta \tilde{x}^{\mu} / \partial x^{\beta}$ is given explicitly at the close of the preceding paragraph.

The desired coordinate differences Δx^{α} are obtained with the aid of the Taylor series:

$$\Delta x^{\alpha} = \tilde{R}_{\beta}^{\alpha} \Delta \tilde{x}^{\beta} + (1/2) \tilde{\Lambda}_{\beta\gamma}^{\alpha} \Delta \tilde{x}^{\beta} \Delta \tilde{x}^{\gamma} + \dots . \quad (43)$$

It is interesting to note that $\Delta \tilde{x}^{\alpha}$ appears not only in the direct form on the right-hand side of (43), but also in the formation of $\tilde{R}_{\beta}^{\alpha}$, $\tilde{\Lambda}_{\beta\gamma}^{\alpha}$, ... as has been illustrated above. This stems from the design of the Q-surface, involving implicitly the point Q already in the construction of any point \tilde{P} ; the more obvious role of $\Delta \tilde{x}^{\alpha}$, reflected explicitly in (43), is that of "bridging the gap" between \tilde{P} and Q. Another interesting feature of the series (43) is that when it is expressed in terms of the initial partial derivatives, the linear term involves not only A_{β}^{α} but also $\Omega_{\beta\gamma}^{\alpha}$, the quadratic term involves A_{β}^{α} , $\Omega_{\beta\gamma}^{\alpha}$, and $\Phi_{\beta\gamma\delta}^{\alpha}$, etc. If Δx^{α} should be expressed from Δu^{α} , the linear term would involve only A_{β}^{α} (it would read $A_{\beta}^{\alpha} \Delta u^{\beta}$), the quadratic term would involve only $\Omega_{\beta\gamma}^{\alpha}$, etc.

Since the coordinate differences Δu^{α} , corresponding to the parametric corrections, are important quantities to be resolved, it is expedient to compute them before completing the set Δx^{α} (by its subset Δx^L). From the subset Δx^{α} computed via (43), we obtain Δu^{α} as

$$\Delta u^{\alpha} = R_{\beta}^{\alpha} \Delta x^{\beta} + (1/2) \Lambda_{\beta\gamma}^{\alpha} \Delta x^{\beta} \Delta x^{\gamma} + (1/6) \Theta_{\beta\gamma\delta}^{\alpha} \Delta x^{\beta} \Delta x^{\gamma} \Delta x^{\delta} + \dots , \quad (44)$$

whose present form corresponds to that of (43) for the reason explained prior to (39). We can express (44) alternately in terms of A_β^α , $\Omega_{\beta\gamma}^\alpha$, $\Phi_{\beta\gamma\delta}^\alpha$, ... as is seen below in (45a,b). In both (44) and (45a,b) the linear term involves only A_β^α , the quadratic term involves only A_β^α and $\Omega_{\beta\gamma}^\alpha$, the cubic term involves A_β^α , $\Omega_{\beta\gamma}^\alpha$, and $\Phi_{\beta\gamma\delta}^\alpha$, etc. To present all three series to within the third-order initial partial derivatives (i.e., $\Phi_{\beta\gamma\delta}^\alpha$), we include an additional term in (44) and (45a) as compared to (43). The alternate expression (45a,b), suitable for programming, is written as

$$\begin{aligned} \Delta u^\alpha = & du^\alpha - (1/2) R_\mu^\alpha (\Omega_{\beta\gamma}^\mu du^\beta du^\gamma) - (1/6) R_\mu^\alpha (\Phi_{\beta\gamma\delta}^\mu du^\beta du^\gamma du^\delta) \\ & - 3 \Omega_{\beta\gamma}^\mu du^\beta R_\eta^\gamma \Omega_{\kappa\tau}^\eta du^\kappa du^\tau - \dots \end{aligned} \quad (45a)$$

where

$$du^\alpha = R_\omega^\alpha \Delta x^\omega \quad (45b)$$

Finally, the remaining subset to be resolved is found from the simplest of the four series:

$$\Delta x^L = A_\beta^L \Delta u^\beta + (1/2) \Omega_{\beta\gamma}^L \Delta u^\beta \Delta u^\gamma + (1/6) \Phi_{\beta\gamma\delta}^L \Delta u^\beta \Delta u^\gamma \Delta u^\delta + \dots \quad (46)$$

which corresponds to (1a) limited to the last $n-u$ coordinate differences. The model-surface coordinates of the least-squares point \bar{P} are $u^\alpha + \Delta u^\alpha$, while its observational-space coordinates are $x^r + \Delta x^r$, where the former corresponds to the adjusted parameters, and the latter, to the adjusted observations. One could verify the consistency of the derivations and the accuracy of the computations by re-evaluating Δx^α , this time based on Δu^α :

$$\Delta x^\alpha = A_\beta^\alpha \Delta u^\beta + (1/2) \Omega_{\beta\gamma}^\alpha \Delta u^\beta \Delta u^\gamma + (1/6) \Phi_{\beta\gamma\delta}^\alpha \Delta u^\beta \Delta u^\gamma \Delta u^\delta + \dots ;$$

the series corresponds to (1a) limited to the first u coordinate differences. All of the observational-space coordinates of \bar{P} could be verified by using (4).

We remark that the parametric resolution via (44) can be by-passed, and the subset Δx^L can be computed by means other than (46). Based on Δx^α found in (43), we have

$$\Delta x^K = -N_\alpha^K \Delta x^\alpha - (1/2) N_{\alpha\beta}^K \Delta x^\alpha \Delta x^\beta - (1/6) N_{\alpha\beta\gamma}^K \Delta x^\alpha \Delta x^\beta \Delta x^\gamma - \dots$$

which, with the notation from (45b), is developed as

$$\begin{aligned}
\Delta x^K = & A_{\alpha}^K du^{\alpha} + (1/2) \{ N_{\mu}^K (\Omega_{\beta\gamma}^{\mu} du^{\beta} du^{\gamma}) + \Omega_{\beta\gamma}^K du^{\beta} du^{\gamma} \} \\
& + (1/6) N_{\mu}^K [(\Phi_{\beta\gamma\delta}^{\mu} du^{\beta} du^{\gamma} du^{\delta} - 3 \Omega_{\beta\gamma}^{\mu} du^{\beta} R_{\eta}^{\gamma} \Omega_{\kappa\tau}^{\eta} du^{\kappa} du^{\tau}) \\
& + \Phi_{\beta\gamma\delta}^K du^{\beta} du^{\gamma} du^{\delta} - 3 \Omega_{\beta\gamma}^K du^{\beta} R_{\eta}^{\gamma} (\Omega_{\kappa\tau}^{\eta} du^{\kappa} du^{\tau})] + \dots \quad (46')
\end{aligned}$$

The expressions written here in parentheses are identical to their counterparts in (45a); their storing can be useful when both Δu^{α} and Δx^K are to be computed.

5. VARIANCE-COVARIANCES AND OTHER ADJUSTMENT QUANTITIES

We now turn to the task of finding the associated metric tensor $\bar{a}^{\alpha\beta}$ and the "necessary" (or restricted) associated metric tensors $\bar{g}^{\prime rs}$ and \bar{g}''^{rs} , where the overbar implies the evaluation at the least-squares point \bar{P} . The first of these tensors belongs to the u -dimensional model surface embedded in the n -dimensional observational space, and corresponds to the variance-covariance matrix of adjusted parameters. The second tensor belongs to the observational space restricted to the u -dimensional hyperplane tangent to the model surface at \bar{P} , and corresponds to the variance-covariance matrix of adjusted observations. And the third tensor belongs to the observational space restricted to the $n-u$ dimensional subspace orthogonal to this hyperplane, and corresponds to the variance-covariance matrix of residuals. The orthogonal subspace just mentioned will be referred to as an $n-u$ dimensional "complementary hyperplane". At the point \bar{P} , we have

$$\bar{g}^{rs} = \bar{g}'^{rs} + \bar{g}''^{rs} ,$$

where \bar{g}^{rs} is the observational-space associated metric tensor corresponding to the variance-covariance matrix of observations. Although \bar{g}^{rs} is considered to be constant for any location in the observational space (see Chapter 2), the same cannot be said about \bar{g}'^{rs} and \bar{g}''^{rs} , which depend on the location of \bar{P} .

The present approach will by-pass the formation of $\bar{a}_{\alpha\beta}$, the model-surface metric tensor at \bar{P} , which would correspond to the weight matrix of adjusted parameters, or, equivalently, to the matrix of normal equations updated for \bar{P} . Likewise, it will by-pass the formation of $\bar{g}_{rs} = g_{rs}$, the observational-space metric tensor, which would correspond to the (constant) weight matrix of observations. Due to the fact that

$$\bar{a}_{\alpha\beta} \bar{a}^{\beta\gamma} = \delta_{\alpha}^{\gamma} , \quad g_{rs} g^{st} = \delta_r^t ,$$

which, in matrix notation are equivalent to

$$[\bar{a}_{\alpha\beta}] = [\bar{a}^{\beta\gamma}]^{-1} , \quad [g_{rs}] = [g^{st}]^{-1} ,$$

it follows that certain matrix inversions will be avoided. For the sake of simplified notation, the desired tensors will be derived for the initial point P , and the resulting formulas will then be applied at the point \bar{P} . We thus

proceed to develop $a^{\alpha\beta}$, g^{rs} , and g'^{rs} , where

$$g'^{rs} = g^{rs} + g''^{rs} . \quad (47)$$

These tensors will be derived in the order g''^{rs} , g^{rs} , and $a^{\alpha\beta}$.

We begin the development by reviewing the notion of the "design tensor" A_α^r appearing, e.g., in Section 3.1 and Appendix B of [Blaha, 1989a]. This tensor can be expressed by means of orthonormal vectors ℓ , j , ... spanning the hyperplane tangent to the model surface at P:

$$A_\alpha^r = \partial x^r / \partial u^\alpha = \ell^r \ell_\alpha + j^r j_\alpha + \dots , \quad (48)$$

with $\{\ell^r\}$, $r=1,2,\dots,n$ representing the observational-space coordinates, and $\{u^\alpha\}$, $\alpha=1,2,\dots,u$ representing the tangent-hyperplane coordinates. The contravariant components of a vector k belonging to the tangent hyperplane transform as

$$k^r = A_\alpha^r k^\alpha . \quad (48')$$

The design tensor (48) can serve in formulating the metric tensor of the tangent hyperplane,

$$a_{\beta\alpha} = \ell_\beta \ell_\alpha + j_\beta j_\alpha + \dots = A_\beta^s g_{sr} A_\alpha^r , \quad (49)$$

as well as the 'necessary' associated metric tensor restricted to the tangent hyperplane,

$$g'^{rs} = \ell^r \ell^s + j^r j^s + \dots = A_\alpha^r a^{\alpha\beta} A_\beta^s , \quad (50)$$

which are both symmetric.

If the independent variables $\{u^\alpha\}$ represent the coordinates for both the tangent hyperplane and the model surface itself, the tensors in (48), (49), and (50) can be used for both these surfaces. However, such equivalencies hold true only at P, whose model-surface coordinates as well as tangent-hyperplane coordinates are u_0^α ; whereas the three tensors are constant in the tangent hyperplane, their values in the model surface change, in general, from point to point (see Appendix B in [Blaha, 1989a]). Since this chapter is concerned only with the values at one point, the conceptual difference between the model surface and the tangent hyperplane can be ignored.

In Chapters 3 and 4 we have seen that the $n-u$ dimensional complementary hyperplane is defined by $n-u$ gradients N_r^L (orthogonal to the model surface), $L=1,2,\dots,n-u$. The set of contravariant components of these $n-u$ gradients are

$$N^{Lr} = g^{rs} N_s^L. \quad (51)$$

We now adopt $\{x^K\}$, $K=1,2,\dots,n-u$ as the coordinates for the complementary hyperplane, and, in analogy to (48) and (49), write A_K^r for its design tensor and a_{KL} for its metric tensor. Thus, in analogy to (48'), if v is a vector belonging to the complementary hyperplane, we have

$$v^r = A_K^r v^K.$$

For a set of $n-u$ vectors v , whose space contravariant components are grouped into N^{Lr} and whose complementary-hyperplane contravariant components are grouped into N^{LM} , it follows that

$$N^{Lr} = A_M^r N^{LM}. \quad (52)$$

If we wish that for each vector v the contravariant components v^R be the same as the last $n-u$ components of v^r , the last $n-u$ coordinates of the system $\{x^r\}$ must be at the same time the complementary-hyperplane coordinates $\{x^K\}$. (In this case, the components of A_K^r are $\{A_K^\rho, \delta_K^R\}$.) This useful provision gives

$$N^{Lr} \equiv \{N^{L\rho}, N^{LR}\}, \quad (53)$$

where N^{Lr} is known from (51). The symbols N^{Lr} and N^{LR} do not represent tensors, but only a collection of $n-u$ contravariant vectors v^r and v^R , respectively.

We next define the symbol M_{KL} such that

$$N^{MJ} M_{JK} = M_{KL} N^{LM} = \delta_K^M, \quad \text{or} \quad [M_{KL}] = [N^{LM}]^{-1}. \quad (54)$$

The combination of (52) and (54) yields

$$\begin{aligned} M_{KL} N^{Lr} &= M_{KL} N^{LM} A_M^r, \\ A_K^r &= M_{KL} N^{Lr}. \end{aligned} \quad (55)$$

(Upon considering equations 53 and 54, this confirms the parenthetical statement from the close of the preceding paragraph.) In analogy to (49), we deduce

$$a_{ML} = A_M^s g_{sr} A_L^r = M_{MJ} N^{Js} g_{sr} N^{Ir} M_{LI}.$$

where

$$N^{Js} g_{sr} N^{Ir} = N^J_r N^{Ir} = N^J_r g^{rs} N^I_s = B^{JI} (-\bar{G}^{IJ}) ,$$

hence

$$a_{ML} = M_{MJ} B^{JI} M_{LI} . \quad (56)$$

Since the associated metric tensor a^{KL} is such that

$$a^{KL} a_{LM} = \delta^K_M , \quad \text{or} \quad [a^{KL}] = [a_{LM}]^{-1} , \quad (57)$$

and since

$$B^{MJ} Q_{JK} = Q_{KL} B^{LM} = \delta^K_M , \quad \text{or} \quad [Q_{KL}] = [B^{LM}]^{-1} ,$$

which has already appeared in a similar form below (41), we deduce:

$$a^{KL} = N^{JK} Q_{JN} N^{NL} . \quad (58)$$

In fact, by contracting this formula with a_{LM} from (56), one recovers equation (57). In analogy to (50), it follows that

$$g^{rs} = A^K_r a^{KL} A^s_L ;$$

the prime has been replaced by the double prime because the role of the tangent hyperplane has been taken by the complementary hyperplane. Upon using equations (55) and (58) in conjunction with (54), this tensor becomes

$$g^{rs} = N^{Jr} Q_{JN} N^{Ns} . \quad (59)$$

We can take advantage of the quantities already found, and formulate g^{rs} in terms of its subsets:

$$g^{\rho\sigma} = N^{J\rho} Q_{JN} N^{N\sigma} , \quad g^{\rho S} = N^{J\rho} Q_{JN} N^{NS} , \quad g^{RS} = N^{JR} Q_{JN} N^{NS} .$$

From (51) we have

$$N^{L\rho} = g^{\rho S} N^L_S = p^{\rho L} , \quad N^{LR} = g^{RS} N^L_S = g^{R\sigma} N^L_\sigma + g^{RL} ;$$

the quantity $p^{\alpha K}$ has appeared below (41) directly, while the result for N^{KM} has participated in forming B^{KM} (ibid.). The subsets of g^{rs} are thus presented as

$$g^{\rho\sigma} = G^\rho_N p^{\sigma N} \quad (= g^{\sigma\rho}) , \quad (60a)$$

$$g^{\rho S} = G^\rho_N N^{NS} \quad (= g^{S\rho}) , \quad (60b)$$

$$g^{RS} = N^{JR} Q_{JN} N^{NS} \quad (= g^{SR}) \quad (60c)$$

From (58) we observe that

$$g^{RS} = a^{RS} \quad (61)$$

This kind of equivalence arises whenever a hyperplane's coordinates coincide with a set of space coordinates.

Having found g^{RS} , we obtain g'^{rs} from (47):

$$g'^{rs} = g^{rs} - g^{RS} \quad (62)$$

For the first subset of g'^{rs} , it follows that

$$g'^{\rho\sigma} = g^{\rho\sigma} - g^{RS} = g^{\rho\sigma} - G_N^{\rho P \sigma N} \quad (62')$$

Next, we consider $\{x^\alpha\}$ to be a coordinate system for the tangent hyperplane, identical with the first u coordinates of the system $\{x^r\}$. In denoting the tangent-hyperplane associated metric tensor in these coordinates by $\tilde{a}^{\alpha\beta}$, in analogy to (61) one has

$$\tilde{a}^{\rho\sigma} = g'^{\rho\sigma} \quad (63)$$

Whereas $\tilde{a}^{\alpha\beta}$ is the associated metric tensor in the system $\{x^\alpha\}$, we are interested in $a^{\alpha\beta}$, the associated metric tensor in the system $\{u^\alpha\}$. Due to the transformation formula

$$a^{\alpha\beta} = (\partial u^\alpha / \partial x^\rho) \tilde{a}^{\rho\sigma} (\partial u^\beta / \partial x^\sigma) \quad ,$$

where $\partial u^\alpha / \partial x^\rho \equiv R_\rho^\alpha$ has already been employed in (14a), equation (63) together with (62') yields

$$a^{\alpha\beta} = R_\rho^\alpha (g^{\rho\sigma} - G_N^{\rho P \sigma N}) R_\sigma^\beta \quad (64)$$

Thus, at P the desired tensors g^{RS} , g'^{rs} , and $a^{\alpha\beta}$ are given respectively by (59) or (60a-c), by (62), and by (64).

Next we consider $\delta \tilde{x}^r$ from (28), written as

$$\delta \tilde{x}^r = N^{Kr} c_K \quad (65)$$

the two subsets of which are

$$\delta \tilde{x}^\rho = P^{\rho K} c_K \quad , \quad \delta \tilde{x}^R = N^{KR} c_K \quad (65')$$

From (65), the covariant components are

$$\delta \tilde{x}_r = g_{rs} \delta \tilde{x}^s = N_r^L c_L.$$

where the last expression is also given in (21). The square of the magnitude of the vector $\delta \tilde{x}$, i.e., the square of the distance between P and \tilde{P} , is

$$\delta \tilde{s}^2 = \delta \tilde{x}^r \delta \tilde{x}_r = N^{Kr} N_r^L c_K c_L.$$

However, since according to the equation preceding (56) we have $N^{Kr} N_r^L = B^{KL}$, it follows that

$$\delta \tilde{s}^2 = c_K B^{KL} c_L = c_K B^{KL} Q_{LM} W^M.$$

and thus (see the equation below 57):

$$\delta \tilde{s}^2 = c_K W^K. \quad (66)$$

The desired tensors \bar{g}^{rs} , \bar{g}'^{rs} , and $\bar{a}^{\alpha\beta}$ are obtained from their unbarred counterparts in (59) or (60a-c), in (62), and in (64), respectively, upon computing all the pertinent quantities at the least-squares point \bar{P} . That is, after the model-surface coordinates of \bar{P} have been found (denoted here as u^α), the algorithm is re-started, but the computation is limited to the quantities featured below equation (41), beginning with G_L^α . The computation includes also the contravariant vector $\delta \tilde{x}^r$ in (65) or (65'), and the invariant $\delta \tilde{s}^2$ in (66). At the point \bar{P} , these two tensors are denoted $\delta \tilde{x}^{\bar{r}}$ and $\delta \tilde{s}^{\bar{2}}$, respectively, representing the contravariant version of the vector $\bar{P}Q$ and the magnitude squared of this vector. In the adjustment terminology, $\delta \tilde{x}^{\bar{r}}$ corresponds to the minus residuals, $-V$, and $\delta \tilde{s}^{\bar{2}}$ corresponds to the least-squares quadratic form, $V^T P V$. All of the above tensors \bar{g}^{rs} , \bar{g}'^{rs} , $\bar{a}^{\alpha\beta}$, $\delta \tilde{x}^{\bar{r}}$, and $\delta \tilde{s}^{\bar{2}}$ are verified numerically in Appendix A.

6. DISCUSSION

6.1 Relation to the Condition Method

The condition method features adjustable observables without any adjustable parameters present. Its geometrical analogue can be expressed in general by

$$F^L(x^r) = N^L = 0, \quad (67a)$$

where N^L has been inserted for the sake of comparison with the outline in Chapter 3. In fact, from equations (7) and (8) we can present the model developed in this study as

$$F^L(x^r) \equiv x^L - f^L(x^\alpha) = N^L = 0. \quad (67b)$$

The comparison of (67a) and (67b) reveals that the method developed herein could be regarded as a special case of the condition method, in the sense that the set of functions F^L has a very special form. It is thus more conveniently regarded (and treated) as a general version of the parametric method.

In geometric analogy, the parameters have been seen to correspond to the model-surface coordinates $\{u^\alpha\}$, and the observables have been seen to correspond to the observational-space coordinates $\{x^r\}$. The Gauss form of the model surface represents the model relationship between the two sets at a general point:

$$x^r = x^r(u^\alpha).$$

In considering the condition-method formulation $F^L(x^r)=0$, which is independent of any potential parameters, we have

$$\begin{aligned} F^L(x^r) &= F^L(x^r(u^\alpha)) = 0, \\ \partial F^L / \partial u^\alpha &= (\partial F^L / \partial x^r)(\partial x^r / \partial u^\alpha) = 0. \end{aligned}$$

The last equality corresponds to the relationship between the condition method and the parametric method for the same adjustment problem, transcribed in matrix notation as $BA=0$. Here this equality has the form

$$N_{r\alpha}^L \equiv N_{\rho\alpha}^L + N_{R\alpha}^L = 0.$$

With regard to the present model (67b) and its geometrical treatment, we have seen in Chapter 4 that

$$N_{\rho}^L = -A_{\lambda}^L R_{\rho}^{\lambda} , \quad N_R^L = \delta_R^L , \quad R_{\rho}^{\lambda} A_{\alpha}^{\rho} = \delta_{\alpha}^{\lambda} .$$

Thus, the above equality is readily verified:

$$N_r^L A_{\alpha}^r = -A_{\alpha}^L + A_{\alpha}^L \equiv 0 .$$

6.2 Solution for a Linear Model

In a linear model, by definition one has

$$A_{\alpha}^r \equiv \text{constant} \neq 0 ; \quad \Omega_{\alpha\beta}^r \equiv 0 , \quad \Phi_{\alpha\beta\gamma}^r \equiv 0 , \dots$$

The equations from Chapter 4 presented in the preceding paragraph are restated for the insight they offer in the linear context:

$$A_{\lambda}^{\alpha} R_{\kappa}^{\lambda} = \delta_{\kappa}^{\alpha} , \quad \text{or} \quad [R_{\kappa}^{\lambda}] = [A_{\lambda}^{\alpha}]^{-1} ,$$

$$N_{\kappa}^L = -A_{\lambda}^L R_{\kappa}^{\lambda} , \quad N_K^L = \delta_K^L .$$

It is apparent that the gradient set N_r^L is constant and the model surface is a hyperplane. From the construction of the Q-surface it then follows that the latter is a hyperplane parallel to the model surface. Further equations in Chapter 4, such as (18a), (19a), ... now lead to

$$\Lambda_{\kappa\tau}^{\lambda} \equiv 0 , \quad \Theta_{\kappa\tau\omega}^{\lambda} \equiv 0 , \dots$$

and equations (18b), (19b), ... lead to

$$N_{\kappa\tau}^L \equiv 0 , \quad N_{\kappa\tau\omega}^L \equiv 0 , \dots$$

From (41) and the equations below it, together with (39) or (39'), we have

$$\tilde{R}_{\beta}^{\alpha} = \tilde{A}_{\beta}^{\alpha} = \delta_{\beta}^{\alpha} .$$

Since (42) and the equations below it show that $\tilde{\Omega}_{\beta\gamma}^{\mu} dx^{\beta} dx^{\gamma} \equiv 0$ for any dx^{β} , it follows that $\tilde{\Omega}_{\beta\gamma}^{\mu} \equiv 0$. Accordingly, the relations preceding (42) yield

$$\tilde{\Lambda}_{\beta\gamma}^{\alpha} \equiv 0 ,$$

with similar identities holding true also for higher-order partial derivatives. From equation (43), together with (38) and (34), we can now write

$$\Delta x^\alpha = \Delta \tilde{x}^\alpha = \delta x^\alpha - g^{\alpha s} N_s^K Q_{KL} N_m^L \delta x^m ,$$

where the first equality is consistent with the fact that the model surface and the Q surface form two parallel hyperplanes; furthermore, from (44) or (45a,b) we can write

$$\Delta u^\alpha = du^\alpha = R_\beta^\alpha \Delta x^\beta .$$

The remaining subset of Δx^Γ then follows from (46) or (46') as

$$\Delta x^L = A_\beta^L \Delta u^\beta = A_\beta^L R_\alpha^\beta \Delta x^\alpha \equiv -N_\alpha^L \Delta x^\alpha .$$

7. CONCLUSION

The non-iterative approach undertaken in the present study is built on the geometrical concept of the functional form of the model surface, coupled with the new concept of the Q-surface. The geometrical restriction to the model surface corresponds to the restriction making the observables consistent with a given adjustment model. The fact that, in general, the observational point Q does not lie in the model surface corresponds to the realization that actual observations will not satisfy the adjustment model exactly. From the geometric standpoint, the least-squares principle implies that the desired point \bar{P} is the foot-point of a line (straight in the flat observational space) dropped orthogonally from Q onto the model surface. The advantage of the functional form of the model surface stems from the property (illustrated in three dimensions) that if a surface is expressed by $N=\text{constant}$, then the gradient of N is a vector orthogonal to this surface. It is then possible to choose a point in the model surface, sufficiently close to the desired least-squares point \bar{P} , and to determine the amount by which a line orthogonal to the surface at this point misses the "target" Q.

The Q-surface plays a crucial role in the determination of this miss, which is expressed in the Q-surface coordinate differences. Such differences are ultimately transformed into the differences of model-surface coordinates; in adjustment terminology, the latter correspond to the parametric corrections. An intermediate transformation features another set of model-surface coordinates, linked to the Q-surface via a set of gradient vectors. All transformations proceed with the aid of the appropriate Taylor-series expansions containing the first- and higher-order partial derivatives of the observables with respect to the parameters in the (nonlinear) adjustment model.

The outline of the geometric approach to a one-step nonlinear adjustment is presented in Chapter 3, and the development leading to an algorithmic resolution is presented in Chapter 4. The centerpiece of this approach is the Taylor-series equation (43). Its first term contains the first- and second-order partial derivatives mentioned above, and it is derived in detail (see, e.g., equations 39' and 41); the second term contains the first-, second-, and third-order partial derivatives, and it is presented without a derivation (see, e.g., equations 40 and 42); the third term contains the first- through fourth-order

partial derivatives, and although it is not presented here, it is used in the numerical example of Appendix A; higher-order terms could be developed, but, similar to the third term, would be useful only in some special situations. The variance-covariance matrices after adjustment (for adjusted parameters, adjusted observations, and residuals), and other adjustment quantities (residuals and the least-squares quadratic form) are presented in Chapter 5. The aspect of reducing a nonlinear adjustment problem with nonlinear constraints to a nonlinear problem with fewer parameters is presented in Appendix B.

In closing, we summarize the main features of the non-iterative approach developed in this study, and compare them with some of the features of the "geometrical method" and the "extended geometrical method" of [Blaha, 1989a], which are iterative in nature:

- 1) The present approach is based on a new and independent concept featuring the Q-surface. An initial point is not displaced by iterations, but the solution is reached in one step; the accuracy of the solution depends on the number of terms included in the pertinent Taylor-series expansions.

- 2) Although the algorithm developed herein is lengthier than the algorithm for the geometrical and extended geometrical methods of [Blaha, 1989a], the partial derivatives of the observables with respect to the parameters are evaluated at only one point (the initial point mentioned above). That is to say, they need not be re-evaluated at new points as is the case with iterative methods; such a task could require a significant effort, depending on the method and accuracy of evaluation (numerical differentiation, estimation, etc.).

- 3) If the fourth-order partial derivatives are significant, they can be incorporated into the derivations and calculations upon proceeding with the first three terms in equation (43). This is beyond the capability of the extended geometrical method of [Blaha, 1989a], which can utilize up to the third-order partial derivatives, and far beyond the capability of the geometrical method (ibid.), which can only utilize the first-and second-order partial derivatives. (The well known and widely used linearized approach, where only the first-order partial derivatives are utilized, may be severely hampered by the nonlinearity of the adjustment model; in the case of strong nonlinearity coupled with inaccurate initial parametric values and/or large observational errors, the solution sought in an iterative process may diverge.)

4) The potential advantage of the non-iterative approach as discussed in the preceding item is heightened upon considering the first iteration in the extended geometrical method of [Blaha, 1989a], where only the first- and second-order partial derivatives are utilized; it is further heightened with respect to the first iteration in the geometrical method (ibid.), where only the first-order partial derivatives are utilized (similar in this respect to the linearized approach). In some cases, the first iteration could actually worsen the initial parametric values, and could even lead the iterative process astray.

5) In following the theory developed herein, it is possible (albeit tedious) to extend the non-iterative algorithm so that it could eventually utilize even the fifth-order partial derivatives, which might be of interest in some special and difficult cases; this would correspond to proceeding with the first four terms in equation (43).

APPENDIX A

NUMERICAL EXAMPLE

The present numerical example is precisely that of Appendix A in [Blaha, 1989a]. The nonlinear parametric adjustment model is represented by six observables, each expressed by a third-order polynomial in four variables. Thus, the number of observations is six, $n=6$, and the number of parameters is four, $u=4$. In terms of the four parameters u^α , $\alpha=1,2,3,4$, a general observable denoted x is expressed by

$$x = c_\alpha u^\alpha + k_{\alpha\beta} u^\alpha u^\beta + m_{\alpha\beta\gamma} u^\alpha u^\beta u^\gamma,$$

where α ranges from 1 to 4, β ranges from α to 4, and γ ranges from β to 4.

The numerical values of the four c -coefficients (linear), the ten k -coefficients (quadratic), and the twenty m -coefficients (cubic) for all six observables are:

+0.8, +1.2, +0.8, +1.5; +2.3, -1.6, +1.7, +2.0, +1.8, -2.1, +2.1, +1.5,
+2.4, +2.1; -1.1, +0.8, -0.9, -2.1, +1.0, -2.0, +1.5, +2.0, -0.9, -1.2, +0.8,
-1.9, -1.3, +0.9, +1.2, +0.8, -2.1, -1.6, +1.8, +1.1.

+1.7, +2.1, -2.1, +1.6; +1.3, +2.2, +1.0, -2.2, +1.7, +1.7, +2.1, +1.8,
+0.7, +1.6; +1.3, -0.8, -0.9, -2.1, +2.0, +1.2, -1.8, +0.9, -1.3, +1.3, -2.1,
-0.9, +1.5, +0.8, +1.1, +1.7, -2.1, -1.8, +1.2, -1.0.

+1.3, -2.1, +1.7, +2.1; +2.2, +2.3, -2.2, +1.1, +1.2, +2.0, -1.7, +1.5,
+1.9, +1.7; -1.1, -2.0, +1.7, +0.8, +1.0, -2.1, +2.2, +1.2, -1.9, +1.7, -1.4,
-0.8, +0.8, +1.0, -1.1, -0.9, +1.8, -1.4, -0.9, +2.1.

+1.6, +1.0, -2.1, +1.1; -1.7, +2.2, +1.6, -1.6, +1.6, -1.2, +2.1, +2.3,
-2.1, +1.2; -2.2, -0.8, +1.0, -1.2, +0.9, +1.3, -0.8, +2.1, +1.9, +1.2, +0.9,
-1.5, -1.6, -0.8, -1.0, +0.9, -0.9, +2.1, +0.8, -1.3.

+0.9, +2.1, -2.1, +1.8; +1.2, +1.7, +2.2, -1.5, +1.9, +1.3, -2.2, +1.7,
+1.0, +2.3; +1.1, -1.2, -0.9, +1.3, +1.5, +1.0, -0.8, -2.2, +0.8, +1.7, -1.2,
-0.8, +1.1, -2.0, +1.7, -0.9, +0.8, +1.3, -1.8, -1.1.

+1.7, +1.2, +1.7, -1.6; +2.1, +1.6, -1.1, +1.9, +1.6, +1.7, +2.0, +1.2,
+1.6, -1.7; +1.3, +2.1, -1.0, -0.8, +1.2, -2.1, +2.2, -1.6, -1.8, -0.8, +1.9,
+1.2, -0.9, +1.2, +2.0, -1.7, +1.1, +1.0, +0.8, -2.2.

The positive-definite variance-covariance matrix of observations, corresponding to the associated metric tensor g^{rs} , is chosen as

$$[g^{rs}] = \begin{bmatrix} +1.3266 & +0.5254 & +0.3669 & +0.1572 & -0.2667 & -0.0549 \\ . & +1.3457 & -0.0281 & +0.5924 & -0.1448 & +0.5521 \\ . & . & +1.4143 & +0.5144 & +0.3600 & -0.5204 \\ . & . & . & +1.4629 & -0.5604 & +0.4877 \\ . & . & . & . & +1.3930 & -0.1034 \\ . & . & . & . & . & +1.3500 \end{bmatrix} .$$

where the dots denote symmetric elements. The positive-definite weight matrix of observations corresponds to the metric tensor g_{sr} , which can be found from $g^{ks} g_{sr} = \delta_r^k$. However, this tensor is not needed here.

The model-surface coordinates of the least-squares point \bar{P} are chosen as

$$u^\alpha = +1.4, -1.2, +1.3, +1.1 .$$

where the notation \bar{u}^α could have been used instead of u^α . The observables "x" for this point are denoted \bar{x}^r , $r=1,2,\dots,6$; computed from the model (third-order polynomial), they are

$$\bar{x}^r = +4.7956, -4.7901, +33.4396, +0.3331, +22.4658, -11.6899 .$$

The observational point Q is generated from \bar{P} by stipulating the values of $\delta\bar{x}^r$, where $\delta\bar{x}$ is the vector $\bar{P}Q$ (see Fig. 1). Since the latter is orthogonal to the model surface, the (final) residuals correspond to $-\delta\bar{x}^r$. The contravariant vector $\delta\bar{x}^r$ is generated by means of the design tensor A_α^r evaluated at \bar{P} as follows. First, the method of Chapter 4 in [Blaha, 1990] gives the matrix $F \equiv [F' F'']$ grouping the contravariant components of orthonormal vectors spanning the observational space: $\ell^r, j^r, \dots, \nu^r, \dots$; the u vectors ℓ, j, \dots span the model surface, and the $n-u$ vectors ν, \dots are orthogonal to it. The components of ℓ^r, j^r, \dots are grouped into the columns of F' , while the components of ν^r, \dots are grouped into the columns of F'' .

Next, the components of $\delta\bar{x}^r$, corresponding to observational errors which must be recovered by the adjustment, are generated from ν^r , ... as

$$\delta\bar{x}^r = a\nu^r + b\eta^r + \dots$$

Here we have $n-u=2$, and choose $a=10$, $b=35$; F'' (not listed) then yields

$$\delta\bar{x}^r = +3.2193, +22.5470, -10.5862, -1.2758, +24.2738, +14.6805$$

We will use two cases of generated errors: case 2 as above, and case 1 where $a=1.0$, $b=3.5$, and where, accordingly, all the values in $\delta\bar{x}^r$ are scaled down by 10. The least-squares quadratic form corresponds to $\delta\bar{s}^2$, where $\delta\bar{s}$ is the magnitude of the vector \bar{PQ} . In general, we have

$$\delta\bar{s}^2 = \delta\bar{x}^r g_{rs} \delta\bar{x}^s = \delta\bar{x}^r \delta\bar{x}^r = a^2 + b^2 + \dots$$

In the present example, it then follows:

$$\text{case 1} \dots \delta\bar{s}^2 = 1^2 + 3.5^2 = 13.25, \quad (\text{A.1a})$$

$$\text{case 2} \dots \delta\bar{s}^2 = 10^2 + 35^2 = 1325. \quad (\text{A.1b})$$

These values must be recovered as the weighted sum of squares of residuals.

The simulated observations correspond to $\bar{x}^r + \delta\bar{x}^r$, determining the point Q. However, the construction implies that the point \bar{P} , obtained by the orthogonal projection of Q onto the model surface, must be the same for both cases 1 and 2, as well as for any other set $\delta\bar{x}^r$ generated as above. At a general point of the model surface, the model-surface metric tensor $a_{\alpha\beta}$, the "necessary" associated metric tensor g'^{rs} , and the "complementary" tensor g''^{rs} can be found from

$$a_{\alpha\beta} = A_{\alpha}^r g_{rs} A_{\beta}^s, \quad (\text{A.2})$$

$$g'^{rs} = A_{\alpha}^r a^{\alpha\beta} A_{\beta}^s, \quad (\text{A.3})$$

$$g''^{rs} = g^{rs} - g'^{rs}, \quad (\text{A.4})$$

where the model-surface associated metric tensor $a^{\alpha\beta}$ is such that

$$a^{\alpha\beta} a_{\beta\gamma} = \delta_{\gamma}^{\alpha}, \quad \text{or} \quad [a^{\alpha\beta}] = [a_{\beta\gamma}]^{-1}.$$

If, in matrix notation, we identify $[g_{rs}] = g^*$, $[g^{rs}] = g$, $[g'^{rs}] = g'$, $[g''^{rs}] = g''$, $[A_{\alpha}^r] = A$, $[a_{\alpha\beta}] = a^*$, and $[a^{\alpha\beta}] = a$, where we have attributed "*" to (purely) covariant tensors, we have

$$a^* = A^T g^* A, \quad a = (a^*)^{-1}, \quad (A.5a,b)$$

$$g' = A a A^T, \quad g'' = g' + g''', \quad (A.6a,b)$$

In a linear adjustment model, a^* in (A.5a) is the well-known matrix of normal equations, $a = (a^*)^{-1}$ is the variance-covariance matrix of adjusted parameters, g' in (A.6a) is the (singular) variance-covariance matrix of adjusted observations, and g'' is the (singular) variance-covariance matrix of residuals. In terms of geometry, such a model entails constant values of A_α^r and thus also of $a_{\alpha\beta}$, $a^{\alpha\beta}$, g'^{rs} , and g''^{rs} (in addition to constant g^{rs} and g_{rs}). In a nonlinear model, these tensors are variable, and must be evaluated at \bar{P} in order to correspond to adjusted quantities. As is shown in Chapter 3 of [Blaha 1990], alternate formulas for g' and g'' are

$$g' = F' F'^T, \quad g'' = F'' F''^T, \quad (A.7a,b)$$

where, for the same reason, $[F' F''] = F$ must again be evaluated at \bar{P} .

All of the formulas and values listed so far have served merely for verification of the numerical results in the present example; the actual results have been computed according to chapter 5. Thus, when applied at \bar{P} , the formulas (65) or (65') have recovered $\delta \bar{x}^r$ for cases 1 and 2, and equation (66) has recovered (A.1a,b). Similarly, the numerical outcome for $[g''^{rs}]$ computed by (59) or (60a-c) agrees with that obtained from (A.6b) and (A.7b), and the numerical outcome for $[g'^{rs}]$ computed by (62) agrees with that obtained from (A.6a) and (A.7a). Finally, $[a^{\alpha\beta}]$ as computed by (64) agrees with (A.5b), while $[a_{\alpha\beta}]$ has been by-passed (similar in this respect to $[g_{rs}]$). Although the above matrices are associated with the least-squares point \bar{P} , the notation is used without an overbar.

The variance covariance matrix for the adjusted parameters and the variance-covariance matrix for the adjusted observations are listed as follows:

$$[a^{\alpha\beta}] = \begin{bmatrix} +0.009205 & +0.010983 & -0.002919 & +0.005380 \\ . & +0.022411 & -0.010135 & +0.016375 \\ . & . & +0.006404 & -0.009214 \\ . & . & . & +0.016113 \end{bmatrix}.$$

$$[g'^{rs}] = \begin{bmatrix} +0.7973 & -0.1196 & +0.0189 & -0.5035 & +0.0501 & -0.1940 \\ . & +0.2940 & -0.2710 & -0.1372 & -0.1325 & +0.1852 \\ . & . & +1.0619 & +0.0285 & +0.8233 & -0.4773 \\ . & . & . & +0.6167 & -0.0587 & +0.3701 \\ . & . & . & . & +0.6775 & -0.2978 \\ . & . & . & . & . & +1.1668 \end{bmatrix}$$

There is no need to list the variance-covariance matrix for the residuals. This matrix is simply $[g''^{rs}] = [g^{rs}] - [g'^{rs}]$, where $[g^{rs}]$ has been presented numerically at the outset.

As in Appendix A of [Blaha, 1989a], the initial set of parameters is represented by

$$u_0^\alpha = +1.399, -1.201, +1.299, +1.099,$$

describing the initial point P by model-surface coordinates. The observational-space coordinates x_0^r of this point are determined from the model, as are the sets of partial derivatives A_α^r , $\Omega_{\alpha\beta}^r$, and $\Phi_{\alpha\beta\gamma}^r$ (the last set is constant here, and any further set is zero). The above coordinate set u_0^α will be utilized for both cases 1 and 2. Accordingly, in the system $\{u^\alpha\}$ the differences between \bar{P} and P are 0.001 units in each of the four coordinates.

We already saw that in the method dubbed "standard" in Appendix A of [Blaha, 1989a], the successive iterations diverged. Below we recapitulate the pertinent results only for the methods dubbed "geometrical" and "extended geometrical" (ibid.). In the former, we present the worst-case errors in the first three iterations, while in the latter, we present such errors in the first two iterations; errors in subsequent iterations are completely negligible. Immediately following the reviewed values, we list errors resulting from the non-iterative approach developed in the present study. Three results will be listed for cases 1 and 2:

(a) The worst-case error in u^α stemming from the utilization of only the first term on the right-hand side of (43), linked to the development of equation (41); this error is referred to as "1-term".

(b) The worst-case error in u^α stemming from the utilization of the first two terms on the right-hand side of (43), linked to equations (41) and (42), of

which the latter has been listed without derivation; this error is referred to as "2-term".

(c) The worst-case error in u^α stemming from the utilization of the first three terms on the right-hand side of (43), of which the third term has not been presented at all; this error is referred to as "3-term".

According to the above description, the results are presented as

case 1 ... geom.: -2×10^{-4} , $+1 \times 10^{-7}$, -1×10^{-10} ;
 ext. geom.: -3×10^{-5} , -1×10^{-10} ;
 non-iter.: 1-term: $+2 \times 10^{-6}$, 2-term: $+4 \times 10^{-8}$, 3-term: $+1 \times 10^{-10}$;
 case 2 ... geom.: -2×10^{-3} , -1×10^{-5} , $+1 \times 10^{-8}$;
 ext. geom.: -1×10^{-5} , -2×10^{-10} ;
 non-iter.: 1-term: $+3 \times 10^{-5}$, 2-term: -4×10^{-8} , 3-term: -5×10^{-10} .

An additional variation of the present example has also been resolved, where

$$u_0^\alpha = +1.39, -1.21, +1.29, +1.09 .$$

The differences between \bar{P} and P in the system $\{u^\alpha\}$ are now 0.01 units in each of the four coordinates, i.e., ten times larger than previously. This set u_0^α is utilized only in conjunction with the observational errors of case 1. The results can be imagined written to the right of the above case 1; this would allow one to visualize the growth of the worst-case errors in u^α due to a ten-fold increase in observational errors (by looking downwards, i.e., examining the above case 2), or due to a ten-fold increase in "errors" in the initial values u_0^α (by looking to the right). The results stemming from this last variation are

case 1 ... geom.: -3×10^{-3} , $+1 \times 10^{-5}$, $+1 \times 10^{-7}$;
 ext. geom.: -2×10^{-3} , $+4 \times 10^{-6}$;
 non-iter.: 1-term: $+2 \times 10^{-4}$, 2-term: $+3 \times 10^{-5}$, 3-term: $+2 \times 10^{-6}$.

In all three methods ("geom.", "ext. geom.", and "non-iter."), the increase in errors in the initial values u_0^α appears to have much more serious repercussions than the increase in observational errors. In fact, the results in "ext. geom." and "non-iter." seem to be degraded only slightly by the increase in observational errors. Iterations in "geom." and, especially, "ext. geom." are seen to decrease the worst-case errors in u^α more dramatically than the addition of terms in "non-iter.". In the latter case, the order of magnitude of such errors is seen to decrease fairly regularly by an inclusion of additional terms, consistent with the characteristics of an expansion in the Taylor series. However, the above results are skewed in disfavor of the non-iterative method, in that only a third-order polynomial serves as an adjustment model. In such a case, the third-order partial derivatives grouped into $\Phi_{\alpha\beta\gamma}^r$ are constant, and the extended geometrical method, which cannot utilize the fourth- and higher-order partial derivatives, is spared any harmful effects these derivatives could entail. By comparison, the third term (not presented) in the non-iterative method operates with the fourth-order partial derivatives, but the latter are identically zero here.

We can conclude the discussion by stating that if the fourth-order partial derivatives of the observables with respect to the parameters were significant, the quality of the results produced by the non-iterative method would likely improve vis-a-vis the extended geometrical method. The improvement would be more dramatic vis-a-vis the geometrical method, which utilizes only up to the second-order partial derivatives. Such an improvement would manifest itself in yet another respect. This respect comes to light upon considering the very first iteration in the extended geometrical method, in which only the first- and second-order partial derivatives are utilized. Accordingly, the extended geometrical method presents potential danger that the first iteration could actually result in worsening of the initial values u_0^α in some special cases, and could even lead the iterative process astray. With regard to the geometrical method, such potential danger would be heightened because this method treats the first iteration in a linearized fashion, i.e., utilizes only the first-order partial derivatives.

APPENDIX B

PARAMETRIC ELIMINATION DUE TO NONLINEAR CONSTRAINTS

B.1 Initial Parametric Values

In standard adjustment notation, a set of s constraints "G" among u parameters is symbolized by

$$G(X^a) = 0 ,$$

where X^a represents the set (column-vector) of adjusted parameters. The usual approach consists in expanding these constraints in the Taylor series using an initial set of parametric values, symbolized by X^0 . It then follows that

$$G(X^a) = W_c + C X + \dots = 0 ,$$

where

$$W_c = G(X^0) , \quad C = (\partial G / \partial X)_0 ,$$

and where $X = X^a - X^0$ is a set of parametric corrections. The subscript "o" indicates that the matrix C is evaluated using the elements of X^0 . This matrix has the dimensions $s \times u$, while the column vectors W_c and X contain s and u elements, respectively. In a standard (linearized) approach, the terms symbolized above by dots are omitted.

Here, as well as in standard adjustment theory, the constraints are considered independent, in the sense that the constraint matrix C has the full row rank s . However, the standard theory proceeds in general with $W_c \neq 0$. By contrast, the current nonlinear development will benefit from such initial values X^0 for which it holds true that

$$G(X^0) = 0 . \tag{B.1}$$

In this case, only $u-s$ of the u values in X^0 can be chosen independently. Although a set X^0 for which $G(X^0) \neq 0$ would also be acceptable, the computations below, which lead to $G(X^0) = 0$ would eventually have to be performed as well, and the resulting formulas would be more cumbersome and less tractable.

We present an example, in matrix notation, of a simple iterative algorithm leading to $G(X^0)=0$. First, the matrix C is partitioned into $[C_1 \ C_2]$, where the submatrices C_1 and C_2 have the dimensions $s \times (u-s)$ and $s \times s$, respectively. The submatrix C_2 can be considered nonsingular without any loss of generality, since, if needed, the parameters could always be rearranged beforehand for this condition to be satisfied. The vector X^0 is similarly partitioned into the subsets denoted temporarily X_1 and X_2 , which contain $u-s$ and s elements, respectively. The elements of X_1 are chosen and held fixed. The remaining elements, grouped in X_2 , are subject to change. We symbolize their initial choice by X_2^0 to accommodate the iterative indices below. The first iteration yields corrections grouped in ΔX_2^1 , resulting in an improved vector X_2^1 . After an i -th iteration, the improved vector becomes

$$X_2^i = X_2^{i-1} + \Delta X_2^i.$$

If the corrections become negligible and the iterative process is terminated after n iterations, the values in X_2^n are adopted as the elements of X_2 . In joining this vector to the independently chosen vector X_1 , one obtains the desired vector X^0 .

The model before the i -th iteration can be presented as follows:

$$G(X^0) \equiv G(X_1, X_2) = G(X_1, X_2^{i-1}) + C_2^{i-1} (X_2 - X_2^{i-1}) + \dots = 0,$$

resulting in the i -th solution:

$$X_2 - X_2^{i-1} = -(C_2^{i-1})^{-1} G(X_1, X_2^{i-1}) + \dots$$

Upon neglecting the higher-order terms represented by the dots, one writes

$$\Delta X_2^i \equiv X_2^i - X_2^{i-1} = -(C_2^{i-1})^{-1} G(X_1, X_2^{i-1}).$$

If the values in ΔX_2^i are not deemed negligible, the matrix C_2 is updated upon evaluating $\partial G / \partial X_2$ with the new values X_2^i , and is denoted C_2^i . Similarly, one forms an updated vector $G(X_1, X_2^i)$ and proceeds to the iteration $i+1$. After the final X^0 has been computed by this or a different method, an actual nonlinear least-squares adjustment with constraints can take place.

B.2 Model Subsurface

As we have seen in Chapter 2, the nonlinear parametric adjustment model can be written as

$$\begin{aligned} x^r(u^\alpha) = & x^r(u_0^\alpha) + A_\alpha^r \Delta u^\alpha + (1/2) \Omega_{\alpha\beta}^r \Delta u^\alpha \Delta u^\beta + \\ & + (1/6) \Phi_{\alpha\beta\gamma}^r \Delta u^\alpha \Delta u^\beta \Delta u^\gamma + \dots \end{aligned} \quad (B.2a)$$

where

$$\Delta u^\alpha = u^\alpha - u_0^\alpha, \quad (B.2b)$$

with $r=1,2,\dots,n$, $\alpha=1,2,\dots,u$; and where

$$\begin{aligned} A_\alpha^r &= (\partial x^r / \partial u^\alpha)_0, & \Omega_{\alpha\beta}^r &= (\partial^2 x^r / \partial u^\alpha \partial u^\beta)_0, \\ \Phi_{\alpha\beta\gamma}^r &= (\partial^3 x^r / \partial u^\alpha \partial u^\beta \partial u^\gamma)_0, \dots \end{aligned}$$

All lower-case Greek letters vary in the fashion prescribed above for α . A similar convention applies for other kinds of indices as well (lower-case Roman letters, etc.). The subscript "0" indicates the evaluation at the initial point P lying in the model surface.

The s nonlinear constraints joined to this model are represented by

$$G^L(u^\alpha) = 0, \quad (B.3a)$$

where $L=1,2,\dots,s$. This equation can be regarded as the functional form of a surface, generalized to higher dimensions. In referring to (B.1), one also has

$$G^L(u_0^\alpha) = 0, \quad (B.3b)$$

where the values u_0^α , $\alpha=1,2,\dots,u$, are known. The functional form (B.3a) restricts the final least-squares point, whose model-surface coordinates are u^α , to a certain lower-dimensional surface embedded in the model surface. From (B.3b) it follows that the initial point P also belongs to this lower-dimensional surface, which will be called "model subsurface". This is apparent from the right-hand sides of (B.3a,b), which contain the same sets of constants (zeros).

The current development is organized along the following lines. First, the coordinate set $\{u^\alpha\}$, $\alpha=1,2,\dots,u$, is partitioned into $\{u^\Lambda, u^K\}$, $\Lambda=1,2,\dots,u-s$, $K=1,2,\dots,s$. This allows (B.3a) to be written as

$$G^L(u^\Lambda, u^K) = 0, \quad (B.4)$$

representing the functional form of the model subsurface. Subject to the condition stated explicitly in the sequel, (B.4) makes it possible to express the last s coordinates in terms of the first $u-s$ coordinates:

$$u^K = u^K(u^\Lambda). \quad (B.5)$$

Equation (B.5) is the Monge form of the model subsurface embedded in the model surface, where u^Λ , $\Lambda=1,2,\dots,u-s$, are the subsurface coordinates (independent variables). The substitution of (B.5) into (B.4) yields

$$g^L(u^\Lambda) \equiv G^L(u^\Lambda, u^K(u^\Lambda)) = 0, \quad (B.6)$$

which is an identity in the model subsurface. Thus, further identities follow:

$$\partial g^L / \partial u^\Lambda = 0, \quad \partial^2 g^L / \partial u^\Lambda \partial u^\Omega = 0, \quad \partial^3 g^L / \partial u^\Lambda \partial u^\Omega \partial u^\Psi = 0, \dots, \quad (B.7)$$

which will be seen to lead to a relation for $u^K(u^\Lambda)$. In this manner, the parameters u^K , $K=1,2,\dots,s$, will have been effectively eliminated.

Expressed in the Taylor series, (B.3a) reads

$$G^L(u^\alpha) \equiv C_\alpha^L \Delta u^\alpha + (1/2) H_{\alpha\beta}^L \Delta u^\alpha \Delta u^\beta + (1/6) T_{\alpha\beta\gamma}^L \Delta u^\alpha \Delta u^\beta \Delta u^\gamma + \dots = 0,$$

where advantage has been taken of (B.3b), and where

$$C_\alpha^L = (\partial G^L / \partial u^\alpha)_0, \quad H_{\alpha\beta}^L = (\partial^2 G^L / \partial u^\alpha \partial u^\beta)_0, \\ T_{\alpha\beta\gamma}^L = (\partial^3 G^L / \partial u^\alpha \partial u^\beta \partial u^\gamma)_0, \dots$$

In using the partition of $\{u^\alpha\}$ and the symmetry of partial derivatives in the lower indices, one develops this equation as

$$G^L(u^\Lambda, u^K) \equiv C_\Lambda^L \Delta u^\Lambda + C_K^L \Delta u^K + (1/2) (H_{\Lambda\Omega}^L \Delta u^\Lambda \Delta u^\Omega + 2 H_{\Lambda K}^L \Delta u^\Lambda \Delta u^K \\ + H_{KM}^L \Delta u^K \Delta u^M) + (1/6) (T_{\Lambda\Omega\Psi}^L \Delta u^\Lambda \Delta u^\Omega \Delta u^\Psi + 3 T_{\Lambda\Omega K}^L \Delta u^\Lambda \Delta u^\Omega \Delta u^K \\ + 3 T_{\Lambda KM}^L \Delta u^\Lambda \Delta u^K \Delta u^M + T_{KMN}^L \Delta u^K \Delta u^M \Delta u^N) + \dots = 0, \quad (B.8a)$$

where

$$\Delta u^\Lambda = u^\Lambda - u_0^\Lambda, \quad \Delta u^K = u^K - u_0^K, \quad (B.8b)$$

and where u_0^Λ, u_0^K , the model-surface coordinates of P, are known (see the relation B.3b and the statement below it). Equation (B.8a) corresponds to the step represented by (B.4). In evoking (B.5), we next formulate the Taylor series for u^K :

$$\Delta u^K = A_{\Lambda}^{K} \Delta u^\Lambda + (1/2) \Omega_{\Lambda\Omega}^{K} \Delta u^\Lambda \Delta u^\Omega + (1/6) \Phi_{\Lambda\Omega\Psi}^{K} \Delta u^\Lambda \Delta u^\Omega \Delta u^\Psi + \dots, \quad (B.9)$$

where

$$A_{\Lambda}^{K} = (\partial u^K / \partial u^\Lambda)_0, \quad \Omega_{\Lambda\Omega}^{K} = (\partial^2 u^K / \partial u^\Lambda \partial u^\Omega)_0, \\ \Phi_{\Lambda\Omega\Psi}^{K} = (\partial^3 u^K / \partial u^\Lambda \partial u^\Omega \partial u^\Psi)_0, \dots$$

The partial derivatives are again symmetric in the lower indices.

The substitution of (B.9) into (B.8a) in view of the step (B.6) yields after a convenient rearrangement:

$$g^L(u^\Lambda) \equiv (C_{\Lambda}^L + C_K^L A_{\Lambda}^{K}) \Delta u^\Lambda + (1/2) (C_K^L \Omega_{\Lambda\Omega}^{K} + H_{\Lambda\Omega}^L + 2 H_{\Lambda K}^L A_{\Omega}^{K} \\ + H_{KM}^L A_{\Lambda}^{K} A_{\Omega}^{M}) \Delta u^\Lambda \Delta u^\Omega + (1/6) (C_K^L \Phi_{\Lambda\Omega\Psi}^{K} + 3 H_{\Lambda K}^L \Omega_{\Omega\Psi}^{K} \\ + 3 H_{KM}^L A_{\Lambda}^{K} \Omega_{\Omega\Psi}^{M} + T_{\Lambda\Omega\Psi}^L + 3 T_{\Lambda\Omega K}^L A_{\Psi}^{K} + 3 T_{\Lambda KM}^L A_{\Omega}^{K} A_{\Psi}^{M} \\ + T_{KMN}^L A_{\Lambda}^{K} A_{\Omega}^{M} A_{\Psi}^{N}) \Delta u^\Lambda \Delta u^\Omega \Delta u^\Psi + \dots = 0.$$

This identity is immediately confirmed at P. Upon differentiating it in succession with respect to $u^\theta, u^\theta u^\Gamma$, etc., and then rearranging the free and the dummy indices while taking advantage of the symmetries in partial derivatives, in accordance with (B.7) it follows that

$$\partial g^L / \partial u^\Lambda \equiv C_{\Lambda}^L + C_K^L A_{\Lambda}^{K} + [C_K^L \Omega_{\Lambda\Omega}^{K} + H_{\Lambda\Omega}^L + H_{\Lambda K}^L A_{\Omega}^{K} + (H_{\Omega K}^L \\ + H_{KM}^L A_{\Omega}^{M}) A_{\Lambda}^{K}] \Delta u^\Omega + (1/2) [C_K^L \Phi_{\Lambda\Omega\Psi}^{K} + H_{\Lambda K}^L \Omega_{\Omega\Psi}^{K} + T_{\Lambda\Omega\Psi}^L \\ + 2 T_{\Lambda\Omega K}^L A_{\Psi}^{K} + T_{\Lambda KM}^L A_{\Omega}^{K} A_{\Psi}^{M} + 2 (H_{\Omega K}^L + H_{KM}^L A_{\Omega}^{M}) \Omega_{\Lambda\Psi}^{K} \\ + (H_{KM}^L \Omega_{\Omega\Psi}^{M} + T_{\Omega\Psi K}^L + 2 T_{\Omega KM}^L A_{\Psi}^{M} \\ + T_{KMN}^L A_{\Omega}^{M} A_{\Psi}^{N}) A_{\Lambda}^{K}] \Delta u^\Omega \Delta u^\Psi + \dots = 0, \quad (B.10)$$

$$\begin{aligned} \partial^2 g^L / \partial u^\Lambda \partial u^\Omega &\equiv C_K^L \Omega'^K + H_{\Lambda\Omega}^L + H_{\Lambda K}^L A'^K_\Omega + (H_{\Omega K}^L + H_{KM}^L A'^M_\Omega) A'^K_\Lambda \\ &+ \{ C_K^L \Phi'^K_{\Lambda\Omega\Psi} + [\dots] \} \Lambda u^\Psi + \dots = 0 , \end{aligned} \quad (B.11)$$

$$\partial^3 g^L / \partial u^\Lambda \partial u^\Omega \partial u^\Psi \equiv C_K^L \Phi'^K_{\Lambda\Omega\Psi} + [\dots] + \dots = 0 ; \quad (B.12)$$

the expression [...] appearing in (B.11,12) is presented explicitly below as the expression inside the brackets in (B.15).

The evaluation of (B.10-12) at P yields, respectively,

$$A'^J_\Lambda = - D_L^J C_\Lambda^L , \quad (B.13)$$

$$\Omega'^J_{\Lambda\Omega} = - D_L^J [H_{\Lambda\Omega}^L + H_{\Lambda K}^L A'^K_\Omega + (H_{\Omega K}^L + H_{KM}^L A'^M_\Omega) A'^K_\Lambda] , \quad (B.14)$$

$$\begin{aligned} \Phi'^J_{\Lambda\Omega\Psi} &= - D_L^J [H_{\Lambda K}^L \Omega'^K_{\Omega\Psi} + T_{\Lambda\Omega\Psi}^L + T_{\Lambda\Omega K}^L A'^K_\Psi + T_{\Lambda\Psi K}^L A'^K_\Omega + T_{\Lambda KM}^L A'^K_\Omega A'^M_\Psi \\ &+ (H_{\Omega K}^L + H_{KM}^L A'^M_\Omega) \Omega'^K_{\Lambda\Psi} + (H_{\Psi K}^L + H_{KM}^L A'^M_\Psi) \Omega'^K_{\Lambda\Omega} \\ &+ (H_{KM}^L \Omega'^M_{\Omega\Psi} + T_{\Omega\Psi K}^L + T_{\Omega KM}^L A'^M_\Psi + T_{\Psi KM}^L A'^M_\Omega \\ &+ T_{KMN}^L A'^M_\Omega A'^N_\Psi) A'^K_\Lambda] , \end{aligned} \quad (B.15)$$

where

$$D_L^M C_K^L = \delta_K^M .$$

The last equation represents the condition mentioned below (B.4). In matrix notation, this condition states that the matrix $[D_L^M]$ is the inverse of $[C_K^L]$, which in turn implies that the matrix $[C_\Lambda^L C_K^L]$ of dimensions $s \times u$ must have the full row rank s , and, therefore, that the constraints must be linearly independent. In the affirmative, an eventual rearranging of parameters will ensure that the matrix $[C_K^L]$ is regular (i.e., square and nonsingular). This subject has already been discussed in Section B.1, and has led to (B.3b). Upon substituting (B.13-15) and higher-order partial derivatives (not listed) into (B.9), one obtains a relationship for u^K as has been indicated below (B.7).

B.3 Modified Nonlinear Model with a Reduced Number of Parameters

Having expressed the model subsurface in (B.5) via (B.9), we can reduce the number of parameters in the model equation (B.2a) by substituting into it the expression for Δu^K from (B.9). Upon the realization that

$$\begin{aligned} A_{\alpha}^r \Delta u^{\alpha} &= A_{\Lambda}^r \Delta u^{\Lambda} + A_K^r \Delta u^K, \\ \Omega_{\alpha\beta}^r \Delta u^{\alpha} \Delta u^{\beta} &= \Omega_{\Lambda\Omega}^r \Delta u^{\Lambda} \Delta u^{\Omega} + 2 \Omega_{\Lambda K}^r \Delta u^{\Lambda} \Delta u^K + \Omega_{KM}^r \Delta u^K \Delta u^M, \\ \Phi_{\alpha\beta\gamma}^r \Delta u^{\alpha} \Delta u^{\beta} \Delta u^{\gamma} &= \Phi_{\Lambda\Omega\Psi}^r \Delta u^{\Lambda} \Delta u^{\Omega} \Delta u^{\Psi} + 3 \Phi_{\Lambda\Omega K}^r \Delta u^{\Lambda} \Delta u^{\Omega} \Delta u^K \\ &\quad + 3 \Phi_{\Lambda KM}^r \Delta u^{\Lambda} \Delta u^K \Delta u^M + \Phi_{KMN}^r \Delta u^K \Delta u^M \Delta u^N, \end{aligned}$$

this substitution yields

$$\begin{aligned} x^r &= x_0^r + (A_{\Lambda}^r + A_K^r A_{\Lambda}^{'K}) \Delta u^{\Lambda} + (1/2) (\Omega_{\Lambda\Omega}^r + A_K^r \Omega_{\Lambda\Omega}^{'K} \\ &\quad + 2 \Omega_{\Lambda K}^r A_{\Omega}^{'K} + \Omega_{KM}^r A_{\Lambda}^{'K} A_{\Omega}^{'M}) \Delta u^{\Lambda} \Delta u^{\Omega} \\ &\quad + (1/6) (\Phi_{\Lambda\Omega\Psi}^r + A_K^r \Phi_{\Lambda\Omega\Psi}^{'K} + 3 \Omega_{\Lambda K}^r \Omega_{\Omega\Psi}^{'K} + 3 \Omega_{KM}^r A_{\Lambda}^{'K} \Omega_{\Omega\Psi}^{'M} \\ &\quad + 3 \Phi_{\Lambda\Omega K}^r A_{\Psi}^{'K} + 3 \Phi_{\Lambda KM}^r A_{\Omega}^{'K} A_{\Psi}^{'M} \\ &\quad + \Phi_{KMN}^r A_{\Lambda}^{'K} A_{\Omega}^{'M} A_{\Psi}^{'N}) \Delta u^{\Lambda} \Delta u^{\Omega} \Delta u^{\Psi} + \dots, \end{aligned} \quad (B.16)$$

where $A_{\Lambda}^{'K}$, $\Omega_{\Lambda\Omega}^{'K}$, \dots , are known from (B.13-15), etc. The symbols x^r and x_0^r in (B.16) are interpreted as

$$x^r \equiv x^r(u^{\alpha}) = x^r(u^{\Lambda}, u^K(u^{\Lambda})) \equiv \bar{x}^r(u^{\Lambda}),$$

$$x_0^r \equiv x^r(u_0^{\alpha}) = x^r(u_0^{\Lambda}, u^K(u_0^{\Lambda})) \equiv \bar{x}^r(u_0^{\Lambda}),$$

where x_0^r is known.

Equation (B.16) is now reformulated to read

$$\begin{aligned} \bar{x}^r(u^{\Lambda}) &= \bar{x}^r(u_0^{\Lambda}) + \bar{A}_{\Lambda}^r \Delta u^{\Lambda} + (1/2) \bar{\Omega}_{\Lambda\Omega}^r \Delta u^{\Lambda} \Delta u^{\Omega} \\ &\quad + (1/6) \bar{\Phi}_{\Lambda\Omega\Psi}^r \Delta u^{\Lambda} \Delta u^{\Omega} \Delta u^{\Psi} + \dots, \end{aligned} \quad (B.17)$$

where the sets of implicit partial derivatives at P, namely

$$\begin{aligned}\bar{A}_{\Lambda}^r &= (\partial \bar{x}^r / \partial u^{\Lambda})_0, & \bar{\Omega}_{\Lambda\Omega}^r &= (\partial^2 \bar{x}^r / \partial u^{\Lambda} \partial u^{\Omega})_0, \\ \bar{\Phi}_{\Lambda\Omega\Psi}^r &= (\partial^3 \bar{x}^r / \partial u^{\Lambda} \partial u^{\Omega} \partial u^{\Psi})_0, \dots\end{aligned}$$

follow readily from (B.16):

$$\bar{A}_{\Lambda}^r = A_{\Lambda}^r + A_K^r A_{\Lambda}^{\prime K}, \quad (B.18a)$$

$$\bar{\Omega}_{\Lambda\Omega}^r = \Omega_{\Lambda\Omega}^r + A_K^r \Omega_{\Lambda\Omega}^{\prime K} + 2 \Omega_{\Lambda K}^r A_{\Omega}^{\prime K} + \Omega_{KM}^r A_{\Lambda}^{\prime K} A_{\Omega}^{\prime M}, \quad (B.18b)$$

$$\begin{aligned}\bar{\Phi}_{\Lambda\Omega\Psi}^r &= \Phi_{\Lambda\Omega\Psi}^r + A_K^r \Phi_{\Lambda\Omega\Psi}^{\prime K} + 3 \Omega_{\Lambda K}^r \Omega_{\Omega\Psi}^{\prime K} + 3 \Omega_{KM}^r A_{\Lambda}^{\prime K} \Omega_{\Omega\Psi}^{\prime M} \\ &+ 3 \Phi_{\Lambda\Omega K}^r A_{\Psi}^{\prime K} + 3 \Phi_{\Lambda KM}^r A_{\Omega}^{\prime K} A_{\Psi}^{\prime M} + \Phi_{KMN}^r A_{\Lambda}^{\prime K} A_{\Omega}^{\prime M} A_{\Psi}^{\prime N}, \dots\end{aligned} \quad (B.18c)$$

Whereas equation (B.2a) represents a nonlinear model in the parameters u^{α} , $\alpha=1,2,\dots,u$, equation (B.17) represents a nonlinear model in the parameters u^{Λ} , $\Lambda=1,2,\dots,u-s$. In geometrical terms, u^{α} are the model-surface coordinates of the point depicting the unconstrained least-squares solution, and u^{Λ} are the model-subsurface coordinates of the point depicting the constrained least-squares solution. Either solution can be carried out using the geometrical algorithm described in the body of the present study, or the algorithm from [Blaha, 1989a]. However, having eliminated the s parameters u^K , one now has a smaller system to resolve.

In conclusion, in the parametric adjustment model with nonlinear constraints, a point representing the least-squares solution is restricted to lie in the model subsurface, i.e., a surface of smaller dimensions than the model surface in which it is embedded. The geometrical approach leads to the replacement of the model surface by the model subsurface, and to the treatment of the observational point Q with respect to the new surface in the usual manner. Accordingly, the constrained least-squares point is the result of an orthogonal projection of Q onto the model subsurface. In the adjustment terminology, this approach eliminates s of the original u parameters, where s is also the number of constraints. The remaining parameters are resolved by the method of the nonlinear parametric least-squares adjustment without constraints, where all the arrays must be properly modified.

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